

Publication Year	2022
Acceptance in OA	2023-06-01T14:15:09Z
Title	Numerical simulations of radar echoes rule out basal CO2 ice deposits at Ultimi Scopuli, Mars
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Publisher's version (DOI)	10.1016/j.icarus.2022.115163
Handle	http://hdl.handle.net/20.500.12386/34228
Journal	ICARUS
Volume	386

1	Numerical simulations of radar echoes rule out basal CO2 ice deposits at
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Abstract
The principal objective of the radar sounder MARSIS experiment is to look for ice and water in the Martian subsurface.
One particular focus of investigations, since 2005, has been the search for basal liquid water in the south polar
layered deposits (SPLD). Anomalously strong basal echoes detected from four distinct areas at the base of the
deposits at Ultimi Scopuli have been interpreted to indicate the presence of bodies of liquid water in this location,
beneath a 1.5 km thick cover of ice and dust. Other explanations for the bright basal reflections have been proposed,
however, including the possibility of constructive interference in layered media. Here, we test this mechanism through
simulations of MARSIS radar signals propagating in models of CO <sub>2</sub> -H <sub>2</sub> O ice sequences. We then compare the results
to real MARSIS data acquired over Ultimi Scopuli, finding that no CO <sub>2</sub> -H <sub>2</sub> O ice model sequence reproduces the set of
real data. The results of our work have implications in relation to the global $CO_2$ inventory of Mars.

**Keywords:** Mars, SPLD, MARSIS, CO<sub>2</sub> ice, radar.

- 61 **1. Introduction**
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The radar sounder MARSIS (Mars Advanced Radar for Subsurface and Ionospheric Sounding) on board the European Space Agency orbiter Mars Express, has been probing the Martian subsurface since 2005 (Orosei et al., 2015), exploring the global distribution of rock, soil, ice, and liquid water. The instrument operates within the range 1.3-5.5 MHz, transmitting a 1 MHz-bandwidth pulse centered at the frequencies of 1.8, 3, 4 and 5 MHz. Exploration of the Martian subsurface is mostly carried out using the 3 and 4 MHz, or 4 and 5 MHz frequencies, for a nominal depth of investigation of up to 5 km, depending on the electromagnetic properties of the probed material (Picardi et al., 2004).

70 The primary objective for the MARSIS experiment is to look for buried ice and water in the Martian 71 subsurface. It was not until 2018, however, that evidence of bright subsurface reflections originating 1.5 km deep 72 below the surface of Ultimi Scopuli, one of the terminal regions of the South Polar Layered Deposits (SPLD), was obtained (Orosei et al., 2018a) at coordinates 193°E - 81°S. The reflections, much brighter than those detected from 73 74 the surface, were interpreted as originating from basal ponded water or wet sediments distributed on an area approximately 20 km across. The work reignited the scientific debate about the stability of liquid water at the Martian 75 76 polar regions, and specifically at the south pole, where average surface temperatures (Mellon et al., 2004) are estimated to be 162 K. A possible explanation for the water being liquid at these conditions is that it contains a high 77 78 concentration of salts (e.g., perchlorates, chlorides) which are ubiquitous on Mars (Hecht et al., 2009) and have 79 eutectic temperatures as low as 198 K (Pestova et al., 2005). It was subsequently suggested that a high geothermal 80 gradient, such as that produced by a magmatic chamber at depth, is required to reach the eutectic temperatures of 81 concentrated salt solutions at the base of the deposits (Sori and Bramson, 2019). This scenario was disputed, 82 however, on the grounds that there is no evidence of an anomalous geothermal gradient in the region (Lauro et al., 83 2021). Newly acquired MARSIS orbits of the region further revealed other three previously undetected areas of bright 84 reflections, each approximately 10 km across (Lauro et al., 2021). Because laboratory experiments have shown that hypersaline aqueous solutions can form and persist over time at temperatures as low as 123 K, well below their 85 eutectic temperatures (Toner et al., 2014; Primm et al., 2017), a hypersaline origin of the water was deemed to remain 86 87 the most likely explanation for the bright reflections (Lauro et al., 2021). It is however difficult to envisage how large bodies of supercooled brines could have persisted in the natural Martian environment over geological timescales 88 89 (Schroeder and Steinbrügge, 2021; Smith et al., 2021), which remains a significant argument against the liquid brine interpretation. The possibility that bright reflections could be caused by scattering phenomena in a stratified medium 90 was also raised (Hecht et al., 2018). This criticism was however dismissed by Orosei et al. (2018b), who pointed out 91 that they had demonstrated that the strength of the basal echoes at Ultimi Scopuli cannot be explained by multiple 92 reflections. Even though a particular stratigraphic arrangement could produce enhanced basal echoes at one of the 93 94 MARSIS frequencies of detection, it did not do so at the other observation frequencies. Alternative models suggesting that a range of materials, other than bodies of liquid water, could explain the sources of the strong basal echoes, have 95 recently been published by Bierson et al. (2021), and Smith et al. (2021). The merits of all proposed alternative 96 hypotheses have been reviewed by Schroeder and Steinbrügge (2021), who argued that none of the alternatives is 97 98 conclusively incompatible with bodies of liquid water as the source of the bright basal reflections, and that each model 99 opens up questions providing new opportunities for future investigations.

Distinct layers of CO<sub>2</sub> ice have been detected by radar sounder SHARAD surveys of the SPLD (Phillips et al., 2011; Bierson et al., 2016). The layers, up to 1 km thick, are interlayered with thin (typically 10-40 m thick) water ice, and it has been calculated that sublimation of these massive deposits of CO<sub>2</sub> ice would increase the Martian atmospheric pressure by 100% (Bierson et al., 2016). It has been suggested that, if the conditions leading to formation

of the thick CO<sub>2</sub>-H<sub>2</sub>O ice deposits have occurred at other times, during the approximately 100 Myr history of formation 104 105 of the SPLD (Manning et al., 2019), then a specific CO<sub>2</sub> ice layering configuration might produce subsurface reflections of higher intensity than those from the surface. In fact, Lalich et al. (2021a,b) obtained strong simulated 106 radar reflections at 4 MHz frequency, mimicking MARSIS waveform, for a model configuration involving 1-100 m thick 107 basal CO<sub>2</sub> ice layers sandwiching a dusty water ice layer of comparable thickness. Such configuration over the extent 108 of MARSIS bright area, would translate in an average ~ 2% of the current CO<sub>2</sub> atmospheric content. While this 109 specific contribution to the atmospheric volatile budget appears negligible, compounding scenarios involving storage 110 of volatiles within the south polar cap can potentially impact estimates of the Martian volatile budget, with 111 112 consequences on models of Martian climate cycles and atmospheric evolution, and on estimates of the amount of volatiles stored in the Martian crust as part of the geological record. 113

114 The Martian polar caps are the most voluminous exposed reservoirs of volatiles on Mars. It is estimated that, combined, the polar caps store two thirds of the entire water content of the planet (Catling, 2014; Smith et al., 2020; 115 Jakoski, 2021). While climate models have suggested the possibility that the polar layered deposits may also contain 116 significant amounts of CO<sub>2</sub> (Jakoski et al., 1995), estimates based on thermophysical properties of water and CO<sub>2</sub> ices 117 rejected such interpretation (Mellon, 1996). The thin veneer of seasonal and residual solid CO<sub>2</sub> on the surface of the 118 polar caps is effectively counted as part of the atmosphere (Jakosky, 2019). However, geomorphological (Gulick and 119 120 Baker, 1989; Baker et al., 1991; Baker, 2001; Ramirez and Craddock, 2018) and geochemical evidence (Bridges et al., 2019) has been interpreted to indicate that early Mars was warmer and wetter than at present, prompting 121 122 suggestions that a thick CO<sub>2</sub> rich atmosphere existed at the time, to account for greenhouse heating of the planet (Haberle et al., 1994). It has been argued that subsequent loss to space of the CO<sub>2</sub> (and other volatiles) does not fully 123 account for the present-day content of CO<sub>2</sub> in the current thin Martian atmosphere, and that massive quantities of CO<sub>2</sub> 124 ought to be sequestered within one or more geological sinks on Mars (Forget et al., 2013). While deep-seated 125 carbonates could in principle accommodate large volumes of CO<sub>2</sub> (Kahn, 1985; Michalski and Niles, 2010; Wray et al., 126 127 2016; Jakosky, 2019), as is the case on Earth, there is at present no conclusive evidence for a global deep-crustal reservoir of carbonates on Mars (Edwards and Ehlmann, 2015). The discovery of massive deposits of CO<sub>2</sub> ice (Phillips 128 et al., 2011; Bierson et al., 2016) in the South Polar Lavered Deposits (SPLD) by the radar sounder SHARAD, and 129 three-dimensional radar imaging volume calculations suggesting the deposits may contain more than 1.6.104 km<sup>3</sup> of 130 dry ice (Putzig et al., 2018), have thus paved the way for renewed investigations into the possibility of the polar ice 131 132 caps as CO<sub>2</sub> sinks.

The global abundance of CO<sub>2</sub> on Mars is presently unknown. There are some generally accepted points, 133 however, that hold irrespective of the exact abundance and distribution of CO<sub>2</sub> on Mars. Mars had lost most of its CO<sub>2</sub> 134 rich atmosphere by the end of the Noachian (~ 3.7 Ga) (Jakosky, 2019). The rate of input of juvenile gases into the 135 atmosphere through planetary outgassing (i.e., volcanic activity) is not known precisely, but it was higher during the 136 Noachian, waning in the Hesperian, becoming negligible in the Amazonian (Grott et al., 2011), so it would have been 137 insufficient to replenish the lost early atmospheric budget. It is not known how much of the initial Martian atmosphere 138 139 was left by the end of the Noachian (estimates range from ~ 0.1 bar to 1 bar; Catling, 2014), and how much  $CO_2$  had 140 by then already been stored in crustal sinks, though it is clear that the overall trend since has been one of thinning of the atmosphere to the present-day global value of  $\sim$  6 mbar of pressure. If the massive CO<sub>2</sub> ice deposits (Phillips et 141 al., 2011) were to sublimate, they would add to the atmosphere as much as ~0.006 bar of CO<sub>2</sub> (Bierson et al., 2016). 142 Further compounding the contribution (however small) of putative additional reservoirs of CO<sub>2</sub> ice hidden in the SPLD, 143 could potentially impact estimates of the planetary CO<sub>2</sub> budget. 144

Here, we present the results of our comprehensive testing of model simulations against the database of MARSIS data acquired over more than 10 years of surveys of the south polar region. We modeled the propagation behaviour of electromagnetic waves at MARSIS operating frequencies (1.8-5 MHz) under a variety of conditions
involving different configurations of thin layers of solid CO<sub>2</sub>, H<sub>2</sub>O ice and dust. Within the parameter space we
explored, the models do not return values of reflection consistent with the observed MARSIS data. We thus reject the
notion that the bright basal reflections detected at Ultimi Scopuli may indicate the presence of thin layers of CO<sub>2</sub>-ice at
the base of the SPLD.

### 153 2. Geological Setting

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The South Polar Layered Deposits (SPLD), covering most of the Planum Australe of Mars (Fig. 1), form an up 155 to 3.7 km thick (Plaut et al., 2007) stratified unit, composed of pure water ice interlayered with thin dust-rich deposits. 156 157 It has been estimated that the content of dust in the SPLD is ~ 10-15% (Plaut et al., 2007; Zuber et al., 2007), although inhomogeneities in the values of inverted density of the deposits indicate that the dust is not uniformly 158 159 distributed (Li et al., 2012), and that the fraction of dust in the water ice would vary depending on the presence of denser CO<sub>2</sub> ice (Broquet et al., 2021). The layers are directly observed in radar imagery where troughs and scarps cut 160 through the deposits (Milkovich and Plaut, 2008). Owing to the electromagnetic contrast between the values of 161 dielectric permittivity  $\varepsilon$  of ice (3.12; Pettinelli et al., 2015) and dust (> 4; Mattei et al., 2014), layering is also detected 162 by radar sounder observations (Plaut et al., 2006, 2007; Milkovich et al., 2009; Whitten and Campbell, 2018), Lavering 163 of the deposits is thought to reflect differential dust and ice accumulation rates influenced by global climate cycles 164 linked to orbital forcing (e.g., Hvidberg et al., 2012). The deposits decrease in elevation and thickness at the margins, 165 eventually waning and revealing underlying Noachian and Hesperian highlands terrains (Tanaka and Kolb, 2001), 166 overlain by a thin mantle of desiccated or water-ice pore-filled soil (Putzig et al., 2005; Jones et al., 2014). The surface 167 age of the SPLD is 7-100 Ma, based on the impact crater record (Herkenhoff and Plaut, 2000; Koutnik et al., 2002). 168 The age of the lowermost strata of the SPLD sequence is presently undetermined. A detailed geological analysis and 169 170 interpretation of the unconformities observed in Promethei Lingula suggests that the current extent of the SPLD may have started forming no earlier than 250 Ma (Guallini et al., 2018). This estimate is consistent with time-series analysis 171 of HiRISE and CaSSIS stereo-images of the internal structure of the SPLD shown along scarp faces, suggesting that 172 the minimum time of accumulation of the SPLD is 10-30 Myr, resulting in a minimum age of deposition for the basal 173 layers of 17 to 130 Ma (Becerra et al., 2019). 174

The SPLD have been subdivided into three distinct structures (Milkovich and Plaut, 2008): the *Promethei Lingula Layer* Sequence (PLL), the *Bench Forming Layer* Sequence (BFL), and the *Inferred Layer* Sequence (IL). The BFL is the top sequence, geographically located in the central west-northwest portion of the SPLD, where the deposits measure their highest elevations (~ 3500-4500 m). The BFL is covered by thin layers of CO<sub>2</sub> ice (part of the South Polar Residual Cap, SPRC). Underlying the BFL is the PLL, while IL is inferred to be the basal sequence in the west of the deposits. Elsewhere, only the PLL exists (ref. to figs. 18-19, in Milkovich and Plaut, 2008), its lateral extent corresponding to that of Tanaka et al.'s (2014) *Apu* (Amazonian polar undivided) unit (Fig. 1).

The South Polar Residual Cap (SPRC), which is part of geological unit IApc (Fig. 1), straddles the prime 182 183 meridian, approximately between longitudes 250°E-40°E and latitudes 85-90°S. The cap is primarily composed of a high albedo thin (<10 m) layer of CO<sub>2</sub> ice (Byrne and Ingersoll, 2003), with a characteristic «Swiss cheese» 184 appearance (Malin et al., 2001) due to the presence of pits that reveal underlying water ice (Zuber et al., 2007). 185 Observed constant rates of erosion of the pits (Thomas et al., 2013) have been interpreted to point to net loss of CO2 186 from the SPRC, possibly counterbalanced by observed net gain of seasonal water ice (Brown et al., 2014), suggesting 187 orbital effects are responsible for the CO2 and H2O atmosphere-SPRC exchanges. Localized deposits up to 1 km 188 thick, formed by alternating layers of CO<sub>2</sub> ice (each approximately 100 m thick) and H<sub>2</sub>O ice (a few m thick) have also 189

190 been detected (Phillips et al., 2011; Bierson et al., 2016) by the radar sounder SHARAD, in troughs and at the base of 191 scarps of the BFL structural unit, to the west of the location of the inferred rim of the ~ 870 km diameter Noachian impact crater Prometheus Basin (Fig. 1). This suggests a possible relationship between the basal topography in this 192 area, and atmospheric conditions that caused deposition of CO<sub>2</sub> ice here. It has been proposed that H<sub>2</sub>O ice entombs 193 the CO<sub>2</sub> ice layers, thus isolating them from the atmosphere and preventing their erosion (Manning et al., 2019). An 194 alternative hypothesis argues that the deposits are in communication with the atmosphere, and that variations in polar 195 196 incident sunlight from Mars's 100 kyr orbital cycles balance the exchange between CO<sub>2</sub> in the deposits and in the atmosphere. The observed deposits should thus record the last 510 kyr of Martian polar climate history (Buhler et al., 197 198 2021). Observations by SHARAD and MARSIS radars did not detect CO2 ice layers anywhere else in the SPLD 199 (Whitten et al., 2017; Whitten and Campbell, 2018; Khuller and Plaut, 2021).

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Fig. 1. Context map of the south polar region. The map shows the extent of the geological units and geographic features
described in Section 2. The dashed aqua polyline indicates the location of the strong basal reflections detected by Lauro et al.
(2021). The trace of the ground track of the tract of SHARAD orbit 5968-01 traversing the RFZ<sub>3</sub> (Phillips et al., 2011) is shown as a
black dashed line on the south pole residual cap (SPRC). Yellow star: South Pole. Vertical yellow line: prime and anti- meridians.
Dashed white line: approximate position of remnant of rim of Promethei Crater. Lime green polyline: boundary of Amazonian polar
undivided unit (*Apu*). Red polyline: boundary of late Amazonian polar cap unit (*IApc*). A-A': end points of topographic profile A-A'
(orange). B-B': end points of topographic profile B-B' (green). The short light blue segment in topographic profile B-B' indicates the

position and inferred depth of the bright basal reflections. Elevations are blended DEM/DTM (200 m/pixel) from MOLA and HRSC
 data. Geological units are described by Tanaka et al. (2014). Geographic grid interval: 10°. Mapped with JMARS.

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Ultimi Scopuli is a vast terminal region of the deposits, part of the Apu geological unit (Fig. 1) and of the 212 structural PLL sequence. Here, between coordinates 191°E-196°E and 80.3-81.5°S, and at a depth of approximately 213 1.5 km, recent orbiter sounder MARSIS observations (Orosei et al., 2018a; Lauro et al., 2021) revealed the presence 214 of four high permittivity areas, interpreted to be bodies of basal liquid water. The heat flow at the Martian south polar 215 regions is ~ 22-26 mW/m<sup>2</sup> (Grott et al., 2013; Plesa et al., 2018), and there is presently no evidence of an anomalous 216 217 geothermal gradient or localized hot spot (such as a magma chamber, as postulated by Sori and Bramson, 2019), that would plausibly increase the basal temperature. The overburden pressure, estimated to be ~ 6 MPa (considering an 218 219 average density of the SPLD = 1220 kg/m<sup>3</sup>, from Zuber et al., 2007, which is the same as the best fit value published by Broquet et al., 2021, and also consistent with a local value of ~ 1200 kg/m<sup>3</sup>, as inferred from the inverted density 220 map of the SPLD published by Li et al., 2012), would also be insufficient for ice to melt. Therefore, to explain the 221 presence of basal liquid water, Orosei et al. (2018a) suggested that the water may be a perchlorate brine. 222 Subsequently, Lauro et al. (2021) further defended this interpretation, on the grounds that supercooled perchlorate 223 brines have been shown to form and persist at sub-eutectic temperatures (Toner et al., 2014; Primm et al., 2017), 224 within the range of those reasonably expected at the base of the SPLD. The reflections at the base of Ultimi Scopuli 225 are located over a gently sloping basement (Lauro et al., 2021). 226

## 228 **3. Model**

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# 230 3.1. Preliminary Analysis

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The fundamental concept underpinning this study is that the electromagnetic waves locally reflected from 232 interfaces between the layers in a stratified structure, can combine to enhance (constructive interference) or suppress 233 (destructive interference) the overall radar response from a layered structure. As a preliminary analysis, we explored 234 the specific parameter space presented by Lalich et al.'s (2021a) model, consisting of a thin layer of pure water ice 235 sandwiched between two thin layers of CO<sub>2</sub> ice: thus, we modelled the variation of only three parameters, i.e., the 236 237 thickness of each of the three layers. Layer thicknesses greater than a few tens of m dampen resonance effects, because longer propagation paths decrease the likelihood of simultaneous in-phase sum of sinusoids at different 238 frequencies (Supplementary Figure 5, Orosei et al., 2018a). Therefore, we constrained the simulated thickness of 239 each layer to be  $\leq$  100 m. In the field of numerical electromagnetic modelling, spatial discretization is usually set to be 240 less than 1/10 of the wavelength. The shortest wavelength transmitted by MARSIS is 30 m in water ice. Thus, we 241 applied simulated thickness increments of 1 m as our sampling interval, to obtain accurate model stratigraphy 242 responses to the MARSIS pulses. We ran more than one million simulations (101 × 101 × 101) at MARSIS operating 243 frequencies of 3, 4 and 5 MHz, obtaining a complete characterization of the properties of Lalich et al.'s (2021a) model. 244

The highest value of subsurface-to-surface echo power ratio we obtained was 4.7 dB. Because the radar response to the stratigraphy is described by sinusoidal functions, we ruled out the eventuality that we might have missed peaks in the subsurface echo: considering that variations in the radar response between consecutive data points are negligible (a fraction of a decibel at most), the model stratigraphy subsurface-to-surface echo power ratios would never exceed ~ 5 dB, even in the case that the position of our maxima were not exact.

For each frequency, we obtained five well-defined regions in parameter space with subsurface-to-surface radar echo power ratio values > 4 dB (Fig. 2). These regions are specific to each frequency, because constructive

- 252 interference phenomena are primarily controlled by layer thickness / wavelength ratios. Consequently, while basal
- echo powers remain high for small variations of thickness around the local maxima at one frequency, the
- corresponding echo powers at the other two frequencies are lower and much more widely dispersed (Fig. 3). Thus, if
- we take the parameter values corresponding to the maxima found at one frequency as a reference, and calculate the
- subsurface-to-surface echo power ratio differences between this frequency and the other two, these will always favour
- the reference frequency (Fig. 4).



- Fig. 2. Location of strong basal echoes (> 4 dB greater than surface echoes) produced in simulations at 4 MHz, displayed in the parameter space of the model by Lalich et al. (2021a), consisting of three quantities, specifically: the thickness of two CO<sub>2</sub> layers, and of a pure water ice layer sandwiched between them. Simulations at 3 and 5 MHz produce the same pattern, but with local
- 262 maxima in different positions.
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- Fig. 3. Histograms of subsurface-to-surface echo power ratios obtained for simulations (orange) with a bottom CO<sub>2</sub> ice layer of thickness ranging between 8 m and 14 m, a top CO<sub>2</sub> ice layer 9-15 m thick, and an interbedded H<sub>2</sub>O ice layer 9-15 m thick. Blue
- 267 histograms represent real MARSIS observations.



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Fig. 4. Histograms of basal-to-surface echo power ratio differences between pairs of MARSIS operating frequencies (3 and 4 MHz, and 4 and 5 MHz). Simulation conditions are the same as for those in Fig. 3. Blue histograms are for real MARSIS observations.

Our preliminary analysis indicates that the distribution and behavior of subsurface-to-surface echo power ratios simulated in the parameter space as described, contrast sharply with that of real MARSIS data. However, idealized models do not consider possible sources of echo power fluctuations that affect real data, and thus some discussion is needed before a comparison between data and model is attempted.

The model used and discussed by Orosei et al. (2018) is computationally the same used by Lalich et al. (2021a, 2021b), that is the one-dimensional solution of Maxwell equations in a plane parallel stratigraphy. The former model had a simpler stratigraphy compared to the latter, with the SPLD represented as a single homogeneous layer composed of a mixture of H<sub>2</sub>O ice and dust. The model was run varying basal temperature, dust content and basal permittivity. These three parameters controlled the attenuation within the SPLD and the intensity of the reflection at the bottom of the SPLD. The results showed that even for low amounts of dust and basal temperatures, it was necessary to have a high basal reflectivity to produce the observed strong basal echoes.

The model parameters published by Lalich et al. (2021b) are exactly the same, except for the input of single values for dust fraction, basal temperature and basal permittivity. These authors varied the thickness of the layers at the base of the SPLD.

Because of the similarity of the mathematical formulation of the two models, we compared them directly to one another to assess their capability to reproduce MARSIS observations, following the same approach used by Lalich et al. (2021b). For example, Figure 3 in that paper shows reflections produced by a single CO<sub>2</sub> layer model that are as strong as the ones observed by MARSIS, although the authors neglected to specify that their reference values for MARSIS echo power are the medians of observed values, and that normalized echo power can reach values as high as 10 dB (see Figure 4 and S4 in Orosei et al., 2018), well above any value that can be obtained by the single layer model shown in Figure 3.

The capability of the model in Orosei et al. (2018) to produce strong echoes is thus not due to a more complex mathematical implementation or to a greater number of parameters, but to the fact that basal permittivity can have

- higher values than those considered by Lalich et al. (2021a, 2021b). In fact, Orosei et al.'s (2018) model could
  produce basal echoes spanning the full range of observed values (see their Figures 4 and S4), whereas Lalich et al.'s
  (2021a, 2021b) resulted only in a few instances of basal echo power comparable to observations. The purpose of the
  present work is therefore to establish the conditions (if these exist), by which Lalich et al.'s (2021) model reproduces
  the strong radar echoes reported by Orosei et al. (2018). We thus performed comprehensive simulations based on the
  same mathematics, using a range of possible parameters beyond that explored in that earlier work.
- In the following sections, we discuss the sources of variability and error affecting MARSIS observations,
   evaluating their effect to derive a model of the uncertainties that can be applied to model results, for a more realistic
   comparison between simulations and data.
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## 305 3.2 Idealized vs. actual SPLD surface geometry

The assumption of a perfectly flat surface does not prevent the possibility of a comparison with real data, as already shown by Orosei et al. (2018). Furthermore, the subsurface echo power for a given orbit is always normalized to its median value, in order to prevent local minima of surface echo power from producing unrealistically high normalized subsurface echo power values. The choice of using surface median power implies the assumption that the SPLD surface is locally homogeneous, and that surface echo power fluctuations are due to small perturbations of this assumed homogeneity.

To verify if this assumption holds, we need to examine the properties of echo power measured by MARSIS. To this end, we retrieved the same data employed to produce Figure 2 in Orosei et al. (2018) and made publicly available at the time of publication of that paper (Orosei and Cicchetti, 2018). We also produced a simulation of surface echo power similar to those presented and discussed in Orosei et al. (2015). Simulations are used to validate subsurface echo detection by visual comparison: all features present in both the real and simulated radargrams are interpreted as surface clutter, and are therefore excluded from interpretation. A comparison between measurements and simulations for orbit 10737 is shown in Figure 5.

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Fig. 5. Top: MARSIS radargram for orbit 10737 at 4 MHz, redrawn following Orosei et al. (2018), versus the corresponding simulation of surface scattering produced using the MOLA topographic dataset (bottom).

The simulated radargram allows also to estimate surface power fluctuations due to surface roughness alone, sampled at the resolution of the MOLA topographic dataset. A comparison with the measured surface power (both arbitrarily normalized to a 0 dB median power for ease of comparison) is shown in Figure 6: it is clear that surface roughness alone accounts for the surface echo power fluctuations at distances between 50 and 60 km along track, which correspond to the location of the bright subsurface reflector.

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The residual difference between data and simulations can be attributed to several factors, such as: surface roughness at scales below MOLA resolution or variations in near-surface density and composition, but the exact cause is difficult to ascertain with available data. Residual power fluctuations are found to have a standard deviation of less than 1 dB, corresponding to a fluctuation of 0.5 in the value of the relative dielectric constant in the assumption that its median value is comprised between 3 and 4 (typical of SPLD materials). Because of the small uncertainties resulting from this analysis, we consider the ratioing with the median surface power as a reasonable calibration method for subsurface echo power.

Furthermore, a previous analysis of SHARAD echoes by Grima et al. (2012) over this area (called Reference Zone or RZ in the paper because of its flatness) showed that surface reflections are predominantly coherent, implying that scattering is near-specular and thus approximates that of a plane surface. This conclusion is even truer at MARSIS wavelength, as the effect of roughness on scattering does not depend on RMS topographic height, but rather on the ratio between RMS topographic height and the wavelength.

It could be argued that even a small roughness causes a decrease (however small) of the mean power of surface echoes, leading to an overestimation of the subsurface-to-surface echo power ratio. In fact, the opposite is true: electromagnetic models and three-dimensional propagation simulations (e.g., Jonard et al., 2019) demonstrate that the wavefront of the radar pulse penetrating through the subsurface is disrupted more than the echo backscattered at the surface, because it crosses the rough surface twice. Thus, the subsurface to surface echo power ratio calculated assuming no surface roughness effect, should be considered a minimum value, with the real ratio likely higher.

356

355 3.3 Signal distortion and noise

The MARSIS pulse is not an ideal chirp. Its actual shape and power are unknown: in fact, the spectra reported 357 by Jordan et al. (2009) do not include the frequency-dependent effects of antenna gain, because these could not be 358 359 measured on ground owing to the length of the antenna. A test comparing the results obtained using Jordan et al.'s (2009) chirp spectra with those obtained using the ideal chirp, does not demonstrate any significant difference. 360 Therefore, the MARSIS data have been range-compressed using an ideal chirp since the beginning of the mission. 361 362 The range compression is not optimal, with both resolution and signal-to-noise ratio affected. This, however, does not affect the ratio of subsurface to surface echo power. In an abstract mathematical representation, radar sounding can 363 364 be described as the convolution of the radar waveform with the ideal electromagnetic response of the observed scene. In Fourier transform terms, this convolution is the multiplication of the stratigraphy spectral response with a band-365 limited signal spectrum, which clips the spectral response bandwidth and produces a limited resolution time-domain 366 response. All these mathematical operations are linear, so the shape of the pulse spectrum will change the power 367 level of echoes from two different interfaces, but not their ratio, which is the quantity used in this analysis. 368

369 A few available data also point to a possible dependence of gain on temperature, although a full characterization of this effect was never performed, because it was considered to be negligible under the conditions at 370 which MARSIS acquires its observations. Furthermore, MARSIS raw data takes are at most 25 seconds long, which is 371 372 too short a time to produce any significant gain variation. This is further corroborated by the plot of surface echo power shown in Figure 6, which does not show any trend of varying gain across the entire observation. Thus, within the limits 373 of what it is technically possible to ascertain about the causes and extent of non-ideality of range compression in 374 MARSIS, there is no effect that should be considered as introducing a bias in the use of median surface echo power 375 376 as a calibration reference for subsurface echo power.

Plots of the noise level in the observations (Orosei and Cicchetti, 2018) analysed by Orosei et al. (2018) show constant noise level across a single observation, and nearly-constant noise levels across observations at the same frequency (around -5 dB at 3 and 4 MHz and -11 dB at 5 MHz when expressed in uncalibrated digital numbers). The median signal-to-noise ratio is > 20 dB for all observations, exceeding 30 dB.

Interferences caused by the electronics of the Mars Express spacecraft were characterized in the commissioning phase of MARSIS. Limited available documentation shows a correlation with the activity of the HRSC camera, though no systematic analysis has ever been published. Overall, data acquired over the lifetime of the mission show that the combined electromagnetic interferences (EMI) caused by orbiter navigation and experiment instrumentations, have a much smaller effect on the functioning of MARSIS than (for example) on its Mars Reconnaissance Orbiter companion SHARAD. Thus, the operating assumption is that EMI have a negligible effect on the subsurface to surface echo power ratio.

The MARSIS data analyzed by Orosei et al. (2018) consist of near-simultaneous observations at two 388 frequencies, namely 3 and 4 MHz, or 4 and 5 MHz. Thus, it is possible to compute the subsurface to surface echo 389 power ratio at two frequencies for the same observation. Doing so for data in which surface echo power has a 390 standard deviation below 1 dB (as noted in Table S1 in the Supplementary Materials of Orosei et al., 2018), one is left 391 392 only with data at 4 and 5 MHz. The difference between normalized power at those two frequencies has a median 393 value of 1.36 dB, which can be used for a back-of the envelope computation based on equations found in Porcello et al. (1974) to obtain an estimate of the loss tangent (see also Orosei et al., 2020 for the effect of such loss tangent 394 value on SHARAD measurements). The resulting value is approximately 0.03, which is about fifteen times greater 395 396 than the one used by Lalich et al. (2021b). Because this value is affected by a large error (the standard deviation of

the difference between normalized power at the two frequencies is almost 4 dB), we did not use the estimated loss
 tangent in simulations. Instead, we considered a variable attenuation as one of the factors decreasing the measured
 ratio between subsurface and surface power produced by a model.

## 401 3.4 Other factors affecting subsurface to surface echo power ratio

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400

Factors affecting subsurface echo power not included in Orosei et al.'s (2018) models are: surface roughness (as discussed above); subsurface roughness (affecting basal echo intensity only); fraction of the radar footprint covered by the basal reflector (see for example Haynes et al., 2018, for a discussion); signal attenuation within the SPLD due to dielectric losses (as discussed above); signal attenuation within the SPLD due to reflection losses in the thinly layered stratigraphy (see for example Courville et al., 2021, for a detailed modelling of propagation in a layered medium at SHARAD frequencies). Their combined effect is demonstrated by the large dispersion of values observed (Figure 7).

410



411

Fig. 7. Histograms of measured values of subsurface to surface echo power ratio over the bright reflector analysed in Orosei et al.
(2018) at 4 MHz (top) and 5 MHz (bottom).

414

The histograms are asymmetric, with a cut-off at high values and a long tail towards low ones. This characteristic matches the intuitive notion that the intensity of a basal reflection cannot increase indefinitely, and would thus have a maximum possible value obtained when all the factors contributing to decreasing basal echo intensity as discussed above are minimized. Thus, a comparison between simulations and data requires the introduction of a model for the random dispersion of measurements. As it is not possible to quantify separately the importance of each factor contributing to basal echo power attenuation, we derived a model probability density function directly from the data (Fig. 8).

The long left-sided tails of the histograms in Figure 7 are characteristic of generalized extreme value distributions, often used to model the maxima of sequences of random variables. Although this is a heuristic method

- 424 for the selection of the model distribution, it has the merit of matching data histograms better than other parametric
- 425 distributions.
- 426







430 Through the remainder of this paper, we use these best-fit distributions as the template for randomly 431 generating synthetic measurements from models.

432

## 433 3.5. Electromagnetic propagation model

434

The propagation of radar waves across stratified media is described by non-linear equations dependent on 435 the electromagnetic properties and thickness of the layers, as well as the probing frequency. Here, we model 436 electromagnetic behaviour of stratified CO<sub>2</sub> ice and dust-laden H<sub>2</sub>O ice, by assuming a 1D geometry (Lombardo et al., 437 2000; Pettinelli et al., 2003; Kartashov et al., 2004; Nunes and Phillips, 2006; Courville et al., 2021). Specifically, we 438 439 simulate the propagation of radar pulses through twelve idealized models of the SPLD, consisting of sets of perfectly parallel planar interstratified basal layers composed of CO2 ice and H2O ice, where the latter has variable contents of 440 dust. The total thickness of the simulated deposits was set at the value derived through MARSIS radargrams over the 441 442 study area (1.5 km). The material underlying the deposits was set to be basaltic rock. The simulations were run by code adapted from MATLAB<sup>(TM)</sup> scripts publicly available through a public research data repository (Orosei and 443 Cicchetti, 2018). The code computes the complex reflectivity of the layer stack across the range of frequencies within 444 the pulse bandwidth, multiplying it by the signal spectrum and Inverse-Fourier transforming to the time domain. 445 Simulations were run for one, two or three  $CO_2$  ice layers, the lowermost of which is in direct contact with the bedrock, 446 while the remaining ones are separated by layers of H<sub>2</sub>O ice of variable thickness (Fig. 9). CO<sub>2</sub> ice layers are 447



450 Fig. 9. Schematic stratigraphy used in numerical simulations. The model stratigraphy is here shown as a set of planar parallel layers of CO<sub>2</sub> ice (dark blue) and H<sub>2</sub>O ice (light blue), bounded by an upper half space representing the Martian atmosphere (as 451 452 semi-infinite vacuum) and a lower half space representing the Martian bedrock (brown). Simulations are run for one, two or three 453 lossless CO<sub>2</sub> ice layers, the lowermost of which is in direct contact with the bedrock, while the remaining ones are separated by layers of H<sub>2</sub>O ice of variable thickness. The topmost layer of H<sub>2</sub>O ice represents the bulk of the stratigraphy. Layer thicknesses of 454 455 CO2 ice and interlayer dusty water ice range from 0 to up to 100 m, with total deposit thickness = 1.5 km. The red arrow indicates 456 the depth direction (-z). The inverted triangle on top of the sequence indicates the surface of the deposits. The sketch is drawn not 457 to scale. 458

Typically, complex relative dielectric permittivities are strongly dependent on the frequency of the propagating 459 electromagnetic wave and the temperature of the medium. Attenuation of the signal is independent of frequency at 460 461 MARSIS wavelength for pure water ice: we used the empirical formulae reported by Mätzler (1998) for the average surface temperature value of 160 K (Clifford, 1987) taken as a constant across the entire model stratigraphy. We find 462 that the real part of the dielectric permittivity of water ice is 3.11, with loss tangent values between 2.5.10<sup>-8</sup> (3 MHz) 463 and 3.7.10<sup>-8</sup> (5 MHz). The loss tangent of CO<sub>2</sub> ice is not well constrained at the temperature of interest, with 464 extrapolations and upper limits only being reported in the published literature. In our computations therefore, we set it 465 to be = 0, to produce the highest possible subsurface-to-surface echo power ratio values. We did not consider the 466 effect of the complex part of the permittivity of CO<sub>2</sub> on the reflection coefficient, because it is generally assumed to be 467 low ( $\leq 10^{-3}$ ). Computing the Fresnel reflection coefficient at normal incidence for an interface between a layer of CO<sub>2</sub> 468 ice and an underlying bedrock with permittivity values such as those used in the simulations, the results, with and 469 without the inclusion of the imaginary part, differ by < 0.00001. 470

471

472 3.6. Simulations

473

474 To calculate the simulated radar waveforms, in our model stratigraphies we assumed perfectly smooth surfaces, an assumption that holds also for small roughness of the illuminated surface, where "small roughness" is 475 defined (Ulaby et al., 1981) by a height <  $\lambda$  /32, which gives a value of 2.35 m at 4MHz. We considered the 476 477 electromagnetic wave transmitted by the radar having a normal incidence with respect to the model stratified structure (ref. to sketch in Fig. 9), and assumed a 1D-model where the only variation of the electromagnetic properties occurs 478 479 along the z-axis (depth). Furthermore, we assumed spatially homogenous layers with a constant complex dielectric permittivity ( $\varepsilon_i$ ) and thickness ( $h_i$ ). The stratified structure is bounded by two half-spaces representative of the 480 atmosphere and the bedrock. This model is the same adopted in previous work (Orosei et al., 2018a; Lauro et al., 481 2019, Lalich et al., 2021a, 2021b). The received signal y(t) is thus computed as: 482

$$y(t) = \mathcal{F}^{-1}[X(f)R(f)], \tag{1}$$

where  $\mathcal{F}^{-1}$  is the inverse Fourier transform, X(f) is the Fourier transform of the signal transmitted by MARSIS antenna, R(f) is the frequency response ( $\Gamma_1(f)$ ) of the layered structure computed from the recursive scattering function  $\Gamma_i(f)$ : 487

$$R(f) = \Gamma_1(f)$$

$$\Gamma_i(f) = \frac{\rho_i + \Gamma_{i+1} e^{-2jk_{i+1}h_{i+1}}}{1 + \rho_i \Gamma_{i+1} e^{-2jk_{i+1}h_{i+1}}},$$
(3)

488

with  $k_i$  the complex-valued wavenumber of the *i*-th layer, and  $\rho_i$  the Fresnel reflection coefficient at the boundary between layer *i*-1 and *i*, given by:

491

$$\rho_i = \frac{\sqrt{\varepsilon_{i-1}} - \sqrt{\varepsilon_i}}{\sqrt{\varepsilon_{i-1}} + \sqrt{\varepsilon_i}},\tag{4}$$

492

The geometry of the problem is modelled as a layered structure, where the upper and lower half space are the same for each simulation, whereas the assumed stratified layer between the atmosphere and the bedrock changes on the basis of the number of  $CO_2$  ice layers, and the thickness of the layers. The ratio between basal and surface power is determined by considering the ratio between the maximum of the square amplitude of y(t) at a time interval containing the echo return from the surface, and that occurring at a time interval containing the echo return from the upper side of the shallower  $CO_2$  ice layer.

Using a multiprocessor machine, we simulated the three  $CO_2$  layer model for every layer thickness between 0 and 50 m at 1-m intervals for three  $CO_2$  layers and two intervening H<sub>2</sub>O layers, for a total of 51<sup>5</sup> simulations. This allowed us to sample completely the parameter space of the models with two- and three-basal  $CO_2$  layers, and thus to locate and explore the properties of local maxima embedded in the three- and five-parameter spaces respectively. We identified local maxima of subsurface to surface power ratio, both at 4 and 5 MHz, and for each of them we extracted the basal echo power ratio for all simulations whose layers are within 2 m of the thickness of those corresponding to the local maximum, thus simulating the effect of random but limited variation of the stratigraphy.

## 507 4. Results

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To implement a quantitative comparison between data and simulation results, for each local maximum of subsurface to surface echo power ratio we produced the histogram of power values extracted from its neighbourhood, and convolved it with the template distributions shown in Figure 8, obtaining a simulated histogram which represents the global effect of the factors affecting propagation within the SPLD on model results. An example of a synthetic distribution is shown in Figure 10.



Fig. 10. Comparison between the histogram of measured values of subsurface to surface echo power ratio at 4 (left) and 5 MHz (right) with the histogram of model results in the neighbourhood of a given local maximum (see text for details), and with the synthetic histogram of model results produced through the convolution of the histogram of model results with the distribution template shown in Figure 8. The histograms are computed both for model results at 4 and 5 MHz.

515

521 To make a guantitative comparison of model results with data, the synthetic histograms were used to 522 generate a set of random values representing measurements. This was done by taking each histogram bin, and generating a set of uniformly distributed random numbers in an interval corresponding to the bin, whose quantity is 523 proportional to the bin height. Finally, the set of synthetic measurements was compared to actual measurements 524 through a statistical test to determine if the two sets of samples could be produced by the same distribution. We used 525 the two-sample Kolmogorov-Smirnov test (Kolmogorov, 1933; Smirnov, 1939), which is a nonparametric test for the 526 527 null hypothesis that the data in two sets of samples are from the same continuous distribution. It is widely employed in 528 statistics for its robustness and its sensitivity to both location and shape of distributions. The test was performed using the implementation available in the MATLAB<sup>(TM)</sup> proprietary programming language, and setting the significance level 529 for the rejection of the null hypothesis at 5%. 530

A configuration of layers producing a local maximum at one frequency does not result in a local maximum at 531 the other frequency. For this reason, both local maxima at 4 MHz and at 5 MHz had to be considered. Thus, for a 532 given model (either two- or three-CO2 ice layers) we simultaneously tested samples of model results at 4 and 5 MHz 533 extracted for a set of layer thicknesses corresponding to a local peak of basal echo power at either 4 or 5 MHz, and 534 535 for all layer thicknesses within two meters of the one producing the peak. This resulted in four possible combinations of number of layers and frequency of the echo power maximum. We found and tested 487 local maxima at 4 MHz and 536 687 at 5 MHz for the two-layer model, and 2981 local maxima at 4 MHz and 5232 at 5 MHz for the three-layer model. 537 Results are shown in Figure 11. 538



539

Fig. 11. Plots of the asymptotic p-values produced by the Kolmogorov-Smirnov test versus the maximum subsurface to surface
 power ratio of simulated echoes, for models with two- and three-CO<sub>2</sub> ice layers and for local maxima at 4 and 5 MHz. Each point
 represents the probability that model results and MARSIS measurements belong to the same continuous distribution. For each
 tested set of simulations, probabilities are computed both at 4 MHz (dots) and at 5 MHz (crosses).

545 No set of two- and three-layer models resulted in simulated values exceeding the 5% significance level 546 threshold. However, it can be seen in the bottom right plot in Figure 11 that a few layer configurations resulting in a 547 local maximum of basal echo power at 5 MHz approach the 5% threshold. This happens only at 5 MHz (crosses in 548 Fig. 11), while at 4 MHz (dots) the probability remains negligible. This quantitatively confirms the observation that, in a 549 model based on the coherent interference between layers, a configuration capable of producing a constructive 550 interference at one frequency is not capable of doing the same at another frequency.

551 None of the modelled scenarios involving CO<sub>2</sub> ice layers reproduce the distribution of basal echo intensities 552 observed by MARSIS over the bright areas in Ultimi Scopuli. Median values of the simulated basal echo power are 553 lower than those observed in real MARSIS data, and the spread of the simulated values does not match the range of 554 the measured data. We thus conclude that the interpretation that best reconciles all radar observations in Ultimi 555 Scopuli remains that of a strong basal reflector overlain by a thick dust-laden SPLD.

556

### 557 5. Conclusions

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The results of our simulations do not support claims that CO2 ice layers interbedded with water ice can 559 produce the bright reflections detected by MARSIS from the base of the SPLD in Ultimi Scopuli. Therefore, we rule out 560 the presence of hidden deposits of basal CO<sub>2</sub> ice in this area. Based on these results, and the lack of detection of 561 sequestered CO2 ice deposits elsewhere in the SPLD (Whitten et al., 2017; Whitten and Campbell, 2018; Khuller and 562 Plaut, 2021) beyond those reported by Phillips et al. (2011) and Bierson et al. (2016), we posit that it is unlikely that 563 hidden  $CO_2$  was stored in the late Amazonian (< 250 Ma) south polar deposits. This conclusion is consistent with the 564 geological record of diminishing volcanic activity on Mars during the Hesperian and throughout the Amazonian, with 565 very small amounts of CO<sub>2</sub> released into the atmosphere by volcanic degassing in post-Noachian times. 566

- 567 With the polar caps being the most voluminous reservoir of volatiles on Mars, and their role in regulating the 568 planetary climate, records of the composition and physical properties of the polar layered deposits are fundamental to 569 constrain the entire geological and climatological history of Mars. The ground penetrating radar MARSIS continuing 570 acquisition of observations over the polar regions is an essential element of our investigations into the origin,
- 571 evolution, and inventory of Martian volatiles and of the planet evolution. This is why interpretations of MARSIS data
- 572 must be critically assessed against the framework of the physical theory of the propagation of radar waves through 573 stratified media, as we have demonstrated in this paper. Rigorous application of this approach to all investigations
- 574 based on MARSIS data will advance our knowledge of the nature and properties of Mars's polar materials.
- 575

## 576 Acknowledgments

577

The authors are grateful to A.P. Rossi and L. Guallini for their helpful comments on an earlier version of this manuscript. We thank two anonymous reviewers for their constructive criticism and insights, that contributed to clarify and improve the paper. This work was supported by the Italian Space Agency (ASI) through contract ASI-INAF 2019– 21-HH.0.

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1	Numerical simulations of radar echoes rule out basal CO2 ice deposits at
2	Ultimi Scopuli, Mars.
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<ul><li>46</li><li>47 Abstract</li></ul>	t
47 Abstract	t
	cipal objective of the radar sounder MARSIS experiment is to look for ice and water in the Martian subsurface
48	cipal objective of the radar sounder MARSIS experiment is to look for ice and water in the Martian subsurface
49 The princ	
50 One part	ticular focus of investigations, since 2005, has been the search for basal liquid water in the south polar
51 layered d	deposits (SPLD). Anomalously strong basal echoes detected from four distinct areas at the base of the
52 deposits	at Ultimi Scopuli have been interpreted to indicate the presence of bodies of liquid water in this location,
53 beneath	a 1.5 km thick cover of ice and dust. Other explanations for the bright basal reflections have been proposed,
54 however,	, including the possibility of constructive interference in layered media. Here, we test this mechanism through
55 simulatio	ons of MARSIS radar signals propagating in models of CO <sub>2</sub> -H <sub>2</sub> O ice sequences. We then compare the results
56 to real M	IARSIS data acquired over Ultimi Scopuli, finding that no CO <sub>2</sub> -H <sub>2</sub> O ice model sequence reproduces the set of
57 real data	a. The results of our work have implications in relation to the global $CO_2$ inventory of Mars.
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59	

**Keywords:** Mars, SPLD, MARSIS, CO<sub>2</sub> ice, radar.

- 61 **1. Introduction**
- 62
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The radar sounder MARSIS (Mars Advanced Radar for Subsurface and Ionospheric Sounding) on board the European Space Agency orbiter Mars Express, has been probing the Martian subsurface since 2005 (Orosei et al., 2015), exploring the global distribution of rock, soil, ice, and liquid water. The instrument operates within the range 1.3-5.5 MHz, transmitting a 1 MHz-bandwidth pulse centered at the frequencies of 1.8, 3, 4 and 5 MHz. Exploration of the Martian subsurface is mostly carried out using the 3 and 4 MHz, or 4 and 5 MHz frequencies, for a nominal depth of investigation of up to 5 km, depending on the electromagnetic properties of the probed material (Picardi et al., 2004).

70 The primary objective for the MARSIS experiment is to look for buried ice and water in the Martian 71 subsurface. It was not until 2018, however, that evidence of bright subsurface reflections originating 1.5 km deep 72 below the surface of Ultimi Scopuli, one of the terminal regions of the South Polar Layered Deposits (SPLD), was obtained (Orosei et al., 2018a) at coordinates 193°E - 81°S. The reflections, much brighter than those detected from 73 74 the surface, were interpreted as originating from basal ponded water or wet sediments distributed on an area approximately 20 km across. The work reignited the scientific debate about the stability of liquid water at the Martian 75 76 polar regions, and specifically at the south pole, where average surface temperatures (Mellon et al., 2004) are estimated to be 162 K. A possible explanation for the water being liquid at these conditions is that it contains a high 77 78 concentration of salts (e.g., perchlorates, chlorides) which are ubiquitous on Mars (Hecht et al., 2009) and have 79 eutectic temperatures as low as 198 K (Pestova et al., 2005). It was subsequently suggested that a high geothermal 80 gradient, such as that produced by a magmatic chamber at depth, is required to reach the eutectic temperatures of 81 concentrated salt solutions at the base of the deposits (Sori and Bramson, 2019). This scenario was disputed, 82 however, on the grounds that there is no evidence of an anomalous geothermal gradient in the region (Lauro et al., 83 2021). Newly acquired MARSIS orbits of the region further revealed other three previously undetected areas of bright 84 reflections, each approximately 10 km across (Lauro et al., 2021). Because laboratory experiments have shown that hypersaline aqueous solutions can form and persist over time at temperatures as low as 123 K, well below their 85 eutectic temperatures (Toner et al., 2014; Primm et al., 2017), a hypersaline origin of the water was deemed to remain 86 the most likely explanation for the bright reflections (Lauro et al., 2021). It is however difficult to envisage how large 87 bodies of supercooled brines could have persisted in the natural Martian environment over geological timescales 88 89 (Schroeder and Steinbrügge, 2021; Smith et al., 2021), which remains a significant argument against the liquid brine interpretation. The possibility that bright reflections could be caused by scattering phenomena in a stratified medium 90 91 was also raised (Hecht et al., 2018). This criticism was however dismissed by Orosei et al. (2018b), who pointed out that they had demonstrated that the strength of the basal echoes at Ultimi Scopuli cannot be explained by multiple 92 reflections. Even though a particular stratigraphic arrangement could produce enhanced basal echoes at one of the 93 94 MARSIS frequencies of detection, it did not do so at the other observation frequencies. Alternative models suggesting that a range of materials, other than bodies of liquid water, could explain the sources of the strong basal echoes, have 95 recently been published by Bierson et al. (2021), and Smith et al. (2021). The merits of all proposed alternative 96 hypotheses have been reviewed by Schroeder and Steinbrügge (2021), who argued that none of the alternatives is 97 98 conclusively incompatible with bodies of liquid water as the source of the bright basal reflections, and that each model 99 opens up questions providing new opportunities for future investigations.

Distinct layers of CO<sub>2</sub> ice have been detected by radar sounder SHARAD surveys of the SPLD (Phillips et al., 2011; Bierson et al., 2016). The layers, up to 1 km thick, are interlayered with thin (typically 10-40 m thick) water ice, and it has been calculated that sublimation of these massive deposits of CO<sub>2</sub> ice would increase the Martian atmospheric pressure by 100% (Bierson et al., 2016). It has been suggested that, if the conditions leading to formation

- 104 of the thick CO<sub>2</sub>-H<sub>2</sub>O ice deposits have occurred at other times, during the approximately 100 Myr history of formation 105 of the SPLD (Manning et al., 2019), then a specific CO<sub>2</sub> ice layering configuration might produce subsurface reflections of higher intensity than those from the surface. In fact, Lalich et al. (2021a,b) obtained strong simulated 106 radar reflections at 4 MHz frequency, mimicking MARSIS waveform, for a model configuration involving 1-100 m thick 107 basal CO<sub>2</sub> ice layers sandwiching a dusty water ice layer of comparable thickness. Such configuration over the extent 108 of MARSIS bright area, would translate in an average ~ 2% of the current CO<sub>2</sub> atmospheric content. While this 109 specific contribution to the atmospheric volatile budget appears negligible, compounding scenarios involving storage 110 of volatiles within the south polar cap can potentially impact estimates of the Martian volatile budget, with 111 112 consequences on models of Martian climate cycles and atmospheric evolution, and on estimates of the amount of volatiles stored in the Martian crust as part of the geological record. 113
- 114 The Martian polar caps are the most voluminous exposed reservoirs of volatiles on Mars. It is estimated that, combined, the polar caps store two thirds of the entire water content of the planet (Catling, 2014; Smith et al., 2020; 115 Jakoski, 2021). While climate models have suggested the possibility that the polar layered deposits may also contain 116 significant amounts of CO<sub>2</sub> (Jakoski et al., 1995), estimates based on thermophysical properties of water and CO<sub>2</sub> ices 117 rejected such interpretation (Mellon, 1996). The thin veneer of seasonal and residual solid CO<sub>2</sub> on the surface of the 118 polar caps is effectively counted as part of the atmosphere (Jakosky, 2019). However, geomorphological (Gulick and 119 120 Baker, 1989; Baker et al., 1991; Baker, 2001; Ramirez and Craddock, 2018) and geochemical evidence (Bridges et al., 2019) has been interpreted to indicate that early Mars was warmer and wetter than at present, prompting 121 122 suggestions that a thick CO<sub>2</sub> rich atmosphere existed at the time, to account for greenhouse heating of the planet (Haberle et al., 1994). It has been argued that subsequent loss to space of the CO<sub>2</sub> (and other volatiles) does not fully 123 account for the present-day content of CO<sub>2</sub> in the current thin Martian atmosphere, and that massive quantities of CO<sub>2</sub> 124 ought to be sequestered within one or more geological sinks on Mars (Forget et al., 2013). While deep-seated 125 carbonates could in principle accommodate large volumes of CO<sub>2</sub> (Kahn, 1985; Michalski and Niles, 2010; Wray et al., 126 127 2016; Jakosky, 2019), as is the case on Earth, there is at present no conclusive evidence for a global deep-crustal reservoir of carbonates on Mars (Edwards and Ehlmann, 2015). The discovery of massive deposits of CO<sub>2</sub> ice (Phillips 128 et al., 2011; Bierson et al., 2016) in the South Polar Layered Deposits (SPLD) by the radar sounder SHARAD, and 129 three-dimensional radar imaging volume calculations suggesting the deposits may contain more than 1.6.104 km<sup>3</sup> of 130 dry ice (Putzig et al., 2018), have thus paved the way for renewed investigations into the possibility of the polar ice 131 132 caps as CO<sub>2</sub> sinks.
- The global abundance of CO<sub>2</sub> on Mars is presently unknown. There are some generally accepted points, 133 however, that hold irrespective of the exact abundance and distribution of CO<sub>2</sub> on Mars. Mars had lost most of its CO<sub>2</sub> 134 rich atmosphere by the end of the Noachian (~ 3.7 Ga) (Jakosky, 2019). The rate of input of juvenile gases into the 135 atmosphere through planetary outgassing (i.e., volcanic activity) is not known precisely, but it was higher during the 136 Noachian, waning in the Hesperian, becoming negligible in the Amazonian (Grott et al., 2011), so it would have been 137 insufficient to replenish the lost early atmospheric budget. It is not known how much of the initial Martian atmosphere 138 139 was left by the end of the Noachian (estimates range from ~ 0.1 bar to 1 bar; Catling, 2014), and how much  $CO_2$  had by then already been stored in crustal sinks, though it is clear that the overall trend since has been one of thinning of 140 the atmosphere to the present-day global value of  $\sim$  6 mbar of pressure. If the massive CO<sub>2</sub> ice deposits (Phillips et 141 al., 2011) were to sublimate, they would add to the atmosphere as much as ~0.006 bar of CO<sub>2</sub> (Bierson et al., 2016). 142 Further compounding the contribution (however small) of putative additional reservoirs of CO<sub>2</sub> ice hidden in the SPLD, 143 could potentially impact estimates of the planetary CO<sub>2</sub> budget. 144
- Here, we present the results of our comprehensive testing of model simulations against the database of
   MARSIS data acquired over more than 10 years of surveys of the south polar region. We modeled the propagation

behaviour of electromagnetic waves at MARSIS operating frequencies (1.8-5 MHz) under a variety of conditions
involving different configurations of thin layers of solid CO<sub>2</sub>, H<sub>2</sub>O ice and dust. Within the parameter space we
explored, the models do not return values of reflection consistent with the observed MARSIS data. We thus reject the
notion that the bright basal reflections detected at Ultimi Scopuli may indicate the presence of thin layers of CO<sub>2</sub>-ice at
the base of the SPLD.

#### 153 2. Geological Setting

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The South Polar Layered Deposits (SPLD), covering most of the Planum Australe of Mars (Fig. 1), form an up 155 to 3.7 km thick (Plaut et al., 2007) stratified unit, composed of pure water ice interlayered with thin dust-rich deposits. 156 157 It has been estimated that the content of dust in the SPLD is ~ 10-15% (Plaut et al., 2007; Zuber et al., 2007), although inhomogeneities in the values of inverted density of the deposits indicate that the dust is not uniformly 158 distributed (Li et al., 2012), and that the fraction of dust in the water ice would vary depending on the presence of 159 denser CO<sub>2</sub> ice (Broquet et al., 2021). The layers are directly observed in radar imagery where troughs and scarps cut 160 through the deposits (Milkovich and Plaut, 2008). Owing to the electromagnetic contrast between the values of 161 dielectric permittivity  $\varepsilon$  of ice (3.12; Pettinelli et al., 2015) and dust (> 4; Mattei et al., 2014), layering is also detected 162 by radar sounder observations (Plaut et al., 2006, 2007; Milkovich et al., 2009; Whitten and Campbell, 2018), Lavering 163 of the deposits is thought to reflect differential dust and ice accumulation rates influenced by global climate cycles 164 linked to orbital forcing (e.g., Hvidberg et al., 2012). The deposits decrease in elevation and thickness at the margins, 165 eventually waning and revealing underlying Noachian and Hesperian highlands terrains (Tanaka and Kolb, 2001), 166 overlain by a thin mantle of desiccated or water-ice pore-filled soil (Putzig et al., 2005; Jones et al., 2014). The surface 167 age of the SPLD is 7-100 Ma, based on the impact crater record (Herkenhoff and Plaut, 2000; Koutnik et al., 2002). 168 The age of the lowermost strata of the SPLD sequence is presently undetermined. A detailed geological analysis and 169 170 interpretation of the unconformities observed in Promethei Lingula suggests that the current extent of the SPLD may have started forming no earlier than 250 Ma (Guallini et al., 2018). This estimate is consistent with time-series analysis 171 of HiRISE and CaSSIS stereo-images of the internal structure of the SPLD shown along scarp faces, suggesting that 172 the minimum time of accumulation of the SPLD is 10-30 Myr, resulting in a minimum age of deposition for the basal 173 layers of 17 to 130 Ma (Becerra et al., 2019). 174

The SPLD have been subdivided into three distinct structures (Milkovich and Plaut, 2008): the *Promethei Lingula Layer* Sequence (PLL), the *Bench Forming Layer* Sequence (BFL), and the *Inferred Layer* Sequence (IL). The BFL is the top sequence, geographically located in the central west-northwest portion of the SPLD, where the deposits measure their highest elevations (~ 3500-4500 m). The BFL is covered by thin layers of CO<sub>2</sub> ice (part of the South Polar Residual Cap, SPRC). Underlying the BFL is the PLL, while IL is inferred to be the basal sequence in the west of the deposits. Elsewhere, only the PLL exists (ref. to figs. 18-19, in Milkovich and Plaut, 2008), its lateral extent corresponding to that of Tanaka et al.'s (2014) *Apu* (Amazonian polar undivided) unit (Fig. 1).

The South Polar Residual Cap (SPRC), which is part of geological unit IApc (Fig. 1), straddles the prime 182 183 meridian, approximately between longitudes 250°E-40°E and latitudes 85-90°S. The cap is primarily composed of a high albedo thin (<10 m) layer of CO<sub>2</sub> ice (Byrne and Ingersoll, 2003), with a characteristic «Swiss cheese» 184 appearance (Malin et al., 2001) due to the presence of pits that reveal underlying water ice (Zuber et al., 2007). 185 Observed constant rates of erosion of the pits (Thomas et al., 2013) have been interpreted to point to net loss of CO2 186 from the SPRC, possibly counterbalanced by observed net gain of seasonal water ice (Brown et al., 2014), suggesting 187 orbital effects are responsible for the CO<sub>2</sub> and H<sub>2</sub>O atmosphere-SPRC exchanges. Localized deposits up to 1 km 188 thick, formed by alternating layers of CO<sub>2</sub> ice (each approximately 100 m thick) and H<sub>2</sub>O ice (a few m thick) have also 189

190 been detected (Phillips et al., 2011; Bierson et al., 2016) by the radar sounder SHARAD, in troughs and at the base of 191 scarps of the BFL structural unit, to the west of the location of the inferred rim of the ~ 870 km diameter Noachian impact crater Prometheus Basin (Fig. 1). This suggests a possible relationship between the basal topography in this 192 area, and atmospheric conditions that caused deposition of CO<sub>2</sub> ice here. It has been proposed that H<sub>2</sub>O ice entombs 193 the CO<sub>2</sub> ice layers, thus isolating them from the atmosphere and preventing their erosion (Manning et al., 2019). An 194 alternative hypothesis argues that the deposits are in communication with the atmosphere, and that variations in polar 195 196 incident sunlight from Mars's 100 kyr orbital cycles balance the exchange between CO<sub>2</sub> in the deposits and in the atmosphere. The observed deposits should thus record the last 510 kyr of Martian polar climate history (Buhler et al., 197 198 2021). Observations by SHARAD and MARSIS radars did not detect CO2 ice layers anywhere else in the SPLD 199 (Whitten et al., 2017; Whitten and Campbell, 2018; Khuller and Plaut, 2021).

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Fig. 1. Context map of the south polar region. The map shows the extent of the geological units and geographic features
described in Section 2. The dashed aqua polyline indicates the location of the strong basal reflections detected by Lauro et al.
(2021). The trace of the ground track of the tract of SHARAD orbit 5968-01 traversing the RFZ<sub>3</sub> (Phillips et al., 2011) is shown as a
black dashed line on the south pole residual cap (SPRC). Yellow star: South Pole. Vertical yellow line: prime and anti- meridians.
Dashed white line: approximate position of remnant of rim of Promethei Crater. Lime green polyline: boundary of Amazonian polar
undivided unit (*Apu*). Red polyline: boundary of late Amazonian polar cap unit (*IApc*). A-A': end points of topographic profile A-A'
(orange). B-B': end points of topographic profile B-B' (green). The short light blue segment in topographic profile B-B' indicates the

position and inferred depth of the bright basal reflections. Elevations are blended DEM/DTM (200 m/pixel) from MOLA and HRSC
 data. Geological units are described by Tanaka et al. (2014). Geographic grid interval: 10°. Mapped with JMARS.

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Ultimi Scopuli is a vast terminal region of the deposits, part of the Apu geological unit (Fig. 1) and of the 212 structural PLL sequence. Here, between coordinates 191°E-196°E and 80.3-81.5°S, and at a depth of approximately 213 1.5 km, recent orbiter sounder MARSIS observations (Orosei et al., 2018a; Lauro et al., 2021) revealed the presence 214 of four high permittivity areas, interpreted to be bodies of basal liquid water. The heat flow at the Martian south polar 215 regions is ~ 22-26 mW/m<sup>2</sup> (Grott et al., 2013; Plesa et al., 2018), and there is presently no evidence of an anomalous 216 217 geothermal gradient or localized hot spot (such as a magma chamber, as postulated by Sori and Bramson, 2019), that would plausibly increase the basal temperature. The overburden pressure, estimated to be ~ 6 MPa (considering an 218 219 average density of the SPLD = 1220 kg/m<sup>3</sup>, from Zuber et al., 2007, which is the same as the best fit value published by Broquet et al., 2021, and also consistent with a local value of ~ 1200 kg/m<sup>3</sup>, as inferred from the inverted density 220 map of the SPLD published by Li et al., 2012), would also be insufficient for ice to melt. Therefore, to explain the 221 presence of basal liquid water, Orosei et al. (2018a) suggested that the water may be a perchlorate brine. 222 Subsequently, Lauro et al. (2021) further defended this interpretation, on the grounds that supercooled perchlorate 223 brines have been shown to form and persist at sub-eutectic temperatures (Toner et al., 2014; Primm et al., 2017), 224 within the range of those reasonably expected at the base of the SPLD. The reflections at the base of Ultimi Scopuli 225 are located over a gently sloping basement (Lauro et al., 2021). 226

## 228 **3. Model**

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# 230 3.1. Preliminary Analysis

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The fundamental concept underpinning this study is that the electromagnetic waves locally reflected from 232 interfaces between the layers in a stratified structure, can combine to enhance (constructive interference) or suppress 233 (destructive interference) the overall radar response from a layered structure. As a preliminary analysis, we explored 234 the specific parameter space presented by Lalich et al.'s (2021a) model, consisting of a thin layer of pure water ice 235 sandwiched between two thin layers of CO<sub>2</sub> ice: thus, we modelled the variation of only three parameters, i.e., the 236 237 thickness of each of the three layers. Layer thicknesses greater than a few tens of m dampen resonance effects, because longer propagation paths decrease the likelihood of simultaneous in-phase sum of sinusoids at different 238 frequencies (Supplementary Figure 5, Orosei et al., 2018a). Therefore, we constrained the simulated thickness of 239 each layer to be  $\leq$  100 m. In the field of numerical electromagnetic modelling, spatial discretization is usually set to be 240 less than 1/10 of the wavelength. The shortest wavelength transmitted by MARSIS is 30 m in water ice. Thus, we 241 applied simulated thickness increments of 1 m as our sampling interval, to obtain accurate model stratigraphy 242 responses to the MARSIS pulses. We ran more than one million simulations (101 × 101 × 101) at MARSIS operating 243 frequencies of 3, 4 and 5 MHz, obtaining a complete characterization of the properties of Lalich et al.'s (2021a) model. 244

The highest value of subsurface-to-surface echo power ratio we obtained was 4.7 dB. Because the radar response to the stratigraphy is described by sinusoidal functions, we ruled out the eventuality that we might have missed peaks in the subsurface echo: considering that variations in the radar response between consecutive data points are negligible (a fraction of a decibel at most), the model stratigraphy subsurface-to-surface echo power ratios would never exceed ~ 5 dB, even in the case that the position of our maxima were not exact.

For each frequency, we obtained five well-defined regions in parameter space with subsurface-to-surface radar echo power ratio values > 4 dB (Fig. 2). These regions are specific to each frequency, because constructive

- 252 interference phenomena are primarily controlled by layer thickness / wavelength ratios. Consequently, while basal
- echo powers remain high for small variations of thickness around the local maxima at one frequency, the
- corresponding echo powers at the other two frequencies are lower and much more widely dispersed (Fig. 3). Thus, if
- we take the parameter values corresponding to the maxima found at one frequency as a reference, and calculate the
- subsurface-to-surface echo power ratio differences between this frequency and the other two, these will always favour
- the reference frequency (Fig. 4).



- Fig. 2. Location of strong basal echoes (> 4 dB greater than surface echoes) produced in simulations at 4 MHz, displayed in the parameter space of the model by Lalich et al. (2021a), consisting of three quantities, specifically: the thickness of two CO<sub>2</sub> layers, and of a pure water ice layer sandwiched between them. Simulations at 3 and 5 MHz produce the same pattern, but with local
- 262 maxima in different positions.
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- Fig. 3. Histograms of subsurface-to-surface echo power ratios obtained for simulations (orange) with a bottom CO<sub>2</sub> ice layer of thickness ranging between 8 m and 14 m, a top CO<sub>2</sub> ice layer 9-15 m thick, and an interbedded H<sub>2</sub>O ice layer 9-15 m thick. Blue
- 267 histograms represent real MARSIS observations.



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Fig. 4. Histograms of basal-to-surface echo power ratio differences between pairs of MARSIS operating frequencies (3 and 4 MHz, and 4 and 5 MHz). Simulation conditions are the same as for those in Fig. 3. Blue histograms are for real MARSIS observations.

Our preliminary analysis indicates that the distribution and behavior of subsurface-to-surface echo power ratios simulated in the parameter space as described, contrast sharply with that of real MARSIS data. However, idealized models do not consider possible sources of echo power fluctuations that affect real data, and thus some discussion is needed before a comparison between data and model is attempted.

The model used and discussed by Orosei et al. (2018) is computationally the same used by Lalich et al. (2021a, 2021b), that is the one-dimensional solution of Maxwell equations in a plane parallel stratigraphy. The former model had a simpler stratigraphy compared to the latter, with the SPLD represented as a single homogeneous layer composed of a mixture of H<sub>2</sub>O ice and dust. The model was run varying basal temperature, dust content and basal permittivity. These three parameters controlled the attenuation within the SPLD and the intensity of the reflection at the bottom of the SPLD. The results showed that even for low amounts of dust and basal temperatures, it was necessary to have a high basal reflectivity to produce the observed strong basal echoes.

The model parameters published by Lalich et al. (2021b) are exactly the same, except for the input of single values for dust fraction, basal temperature and basal permittivity. These authors varied the thickness of the layers at the base of the SPLD.

Because of the similarity of the mathematical formulation of the two models, we compared them directly to one another to assess their capability to reproduce MARSIS observations, following the same approach used by Lalich et al. (2021b). For example, Figure 3 in that paper shows reflections produced by a single CO<sub>2</sub> layer model that are as strong as the ones observed by MARSIS, although the authors neglected to specify that their reference values for MARSIS echo power are the medians of observed values, and that normalized echo power can reach values as high as 10 dB (see Figure 4 and S4 in Orosei et al., 2018), well above any value that can be obtained by the single layer model shown in Figure 3.

The capability of the model in Orosei et al. (2018) to produce strong echoes is thus not due to a more complex mathematical implementation or to a greater number of parameters, but to the fact that basal permittivity can have

- higher values than those considered by Lalich et al. (2021a, 2021b). In fact, Orosei et al.'s (2018) model could
  produce basal echoes spanning the full range of observed values (see their Figures 4 and S4), whereas Lalich et al.'s
  (2021a, 2021b) resulted only in a few instances of basal echo power comparable to observations. The purpose of the
  present work is therefore to establish the conditions (if these exist), by which Lalich et al.'s (2021) model reproduces
  the strong radar echoes reported by Orosei et al. (2018). We thus performed comprehensive simulations based on the
  same mathematics, using a range of possible parameters beyond that explored in that earlier work.
- In the following sections, we discuss the sources of variability and error affecting MARSIS observations,
   evaluating their effect to derive a model of the uncertainties that can be applied to model results, for a more realistic
   comparison between simulations and data.
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## 305 3.2 Idealized vs. actual SPLD surface geometry

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The assumption of a perfectly flat surface does not prevent the possibility of a comparison with real data, as already shown by Orosei et al. (2018). Furthermore, the subsurface echo power for a given orbit is always normalized to its median value, in order to prevent local minima of surface echo power from producing unrealistically high normalized subsurface echo power values. The choice of using surface median power implies the assumption that the SPLD surface is locally homogeneous, and that surface echo power fluctuations are due to small perturbations of this assumed homogeneity.

To verify if this assumption holds, we need to examine the properties of echo power measured by MARSIS. To this end, we retrieved the same data employed to produce Figure 2 in Orosei et al. (2018) and made publicly available at the time of publication of that paper (Orosei and Cicchetti, 2018). We also produced a simulation of surface echo power similar to those presented and discussed in Orosei et al. (2015). Simulations are used to validate subsurface echo detection by visual comparison: all features present in both the real and simulated radargrams are interpreted as surface clutter, and are therefore excluded from interpretation. A comparison between measurements and simulations for orbit 10737 is shown in Figure 5.



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**Fig. 5.** Top: MARSIS radargram for orbit 10737 at 4 MHz, redrawn following Orosei et al. (2018), versus the corresponding simulation of surface scattering produced using the MOLA topographic dataset (bottom).

The simulated radargram allows also to estimate surface power fluctuations due to surface roughness alone, sampled at the resolution of the MOLA topographic dataset. A comparison with the measured surface power (both arbitrarily normalized to a 0 dB median power for ease of comparison) is shown in Figure 6: it is clear that surface roughness alone accounts for the surface echo power fluctuations at distances between 50 and 60 km along track, which correspond to the location of the bright subsurface reflector.

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**Fig. 6.** Measured vs. simulated surface echo power for orbit 10737 at 4 MHz, both arbitrarily normalized to a 0 dB median power for ease of comparison.

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The residual difference between data and simulations can be attributed to several factors, such as: surface roughness at scales below MOLA resolution or variations in near-surface density and composition, but the exact cause is difficult to ascertain with available data. Residual power fluctuations are found to have a standard deviation of less than 1 dB, corresponding to a fluctuation of 0.5 in the value of the relative dielectric constant in the assumption that its median value is comprised between 3 and 4 (typical of SPLD materials). Because of the small uncertainties resulting from this analysis, we consider the ratioing with the median surface power as a reasonable calibration method for subsurface echo power.

Furthermore, a previous analysis of SHARAD echoes by Grima et al. (2012) over this area (called Reference Zone or RZ in the paper because of its flatness) showed that surface reflections are predominantly coherent, implying that scattering is near-specular and thus approximates that of a plane surface. This conclusion is even truer at MARSIS wavelength, as the effect of roughness on scattering does not depend on RMS topographic height, but rather on the ratio between RMS topographic height and the wavelength.

It could be argued that even a small roughness causes a decrease (however small) of the mean power of surface echoes, leading to an overestimation of the subsurface-to-surface echo power ratio. In fact, the opposite is true: electromagnetic models and three-dimensional propagation simulations (e.g., Jonard et al., 2019) demonstrate that the wavefront of the radar pulse penetrating through the subsurface is disrupted more than the echo backscattered at the surface, because it crosses the rough surface twice. Thus, the subsurface to surface echo power ratio calculated assuming no surface roughness effect, should be considered a minimum value, with the real ratio likely higher.

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## 355 3.3 Signal distortion and noise

The MARSIS pulse is not an ideal chirp. Its actual shape and power are unknown: in fact, the spectra reported 357 by Jordan et al. (2009) do not include the frequency-dependent effects of antenna gain, because these could not be 358 359 measured on ground owing to the length of the antenna. A test comparing the results obtained using Jordan et al.'s (2009) chirp spectra with those obtained using the ideal chirp, does not demonstrate any significant difference. 360 Therefore, the MARSIS data have been range-compressed using an ideal chirp since the beginning of the mission. 361 362 The range compression is not optimal, with both resolution and signal-to-noise ratio affected. This, however, does not 363 affect the ratio of subsurface to surface echo power. In an abstract mathematical representation, radar sounding can 364 be described as the convolution of the radar waveform with the ideal electromagnetic response of the observed scene. In Fourier transform terms, this convolution is the multiplication of the stratigraphy spectral response with a band-365 limited signal spectrum, which clips the spectral response bandwidth and produces a limited resolution time-domain 366 367 response. All these mathematical operations are linear, so the shape of the pulse spectrum will change the power level of echoes from two different interfaces, but not their ratio, which is the quantity used in this analysis. 368

369 A few available data also point to a possible dependence of gain on temperature, although a full characterization of this effect was never performed, because it was considered to be negligible under the conditions at 370 which MARSIS acquires its observations. Furthermore, MARSIS raw data takes are at most 25 seconds long, which is 371 372 too short a time to produce any significant gain variation. This is further corroborated by the plot of surface echo power shown in Figure 6, which does not show any trend of varying gain across the entire observation. Thus, within the limits 373 of what it is technically possible to ascertain about the causes and extent of non-ideality of range compression in 374 MARSIS, there is no effect that should be considered as introducing a bias in the use of median surface echo power 375 376 as a calibration reference for subsurface echo power.

Plots of the noise level in the observations (Orosei and Cicchetti, 2018) analysed by Orosei et al. (2018) show constant noise level across a single observation, and nearly-constant noise levels across observations at the same frequency (around -5 dB at 3 and 4 MHz and -11 dB at 5 MHz when expressed in uncalibrated digital numbers). The median signal-to-noise ratio is > 20 dB for all observations, exceeding 30 dB.

Interferences caused by the electronics of the Mars Express spacecraft were characterized in the commissioning phase of MARSIS. Limited available documentation shows a correlation with the activity of the HRSC camera, though no systematic analysis has ever been published. Overall, data acquired over the lifetime of the mission show that the combined electromagnetic interferences (EMI) caused by orbiter navigation and experiment instrumentations, have a much smaller effect on the functioning of MARSIS than (for example) on its Mars Reconnaissance Orbiter companion SHARAD. Thus, the operating assumption is that EMI have a negligible effect on the subsurface to surface echo power ratio.

The MARSIS data analyzed by Orosei et al. (2018) consist of near-simultaneous observations at two 388 frequencies, namely 3 and 4 MHz, or 4 and 5 MHz. Thus, it is possible to compute the subsurface to surface echo 389 power ratio at two frequencies for the same observation. Doing so for data in which surface echo power has a 390 standard deviation below 1 dB (as noted in Table S1 in the Supplementary Materials of Orosei et al., 2018), one is left 391 392 only with data at 4 and 5 MHz. The difference between normalized power at those two frequencies has a median 393 value of 1.36 dB, which can be used for a back-of the envelope computation based on equations found in Porcello et al. (1974) to obtain an estimate of the loss tangent (see also Orosei et al., 2020 for the effect of such loss tangent 394 395 value on SHARAD measurements). The resulting value is approximately 0.03, which is about fifteen times greater 396 than the one used by Lalich et al. (2021b). Because this value is affected by a large error (the standard deviation of

the difference between normalized power at the two frequencies is almost 4 dB), we did not use the estimated loss
 tangent in simulations. Instead, we considered a variable attenuation as one of the factors decreasing the measured
 ratio between subsurface and surface power produced by a model.

## 401 3.4 Other factors affecting subsurface to surface echo power ratio

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Factors affecting subsurface echo power not included in Orosei et al.'s (2018) models are: surface roughness (as discussed above); subsurface roughness (affecting basal echo intensity only); fraction of the radar footprint covered by the basal reflector (see for example Haynes et al., 2018, for a discussion); signal attenuation within the SPLD due to dielectric losses (as discussed above); signal attenuation within the SPLD due to reflection losses in the thinly layered stratigraphy (see for example Courville et al., 2021, for a detailed modelling of propagation in a layered medium at SHARAD frequencies). Their combined effect is demonstrated by the large dispersion of values observed (Figure 7).

410



Fig. 7. Histograms of measured values of subsurface to surface echo power ratio over the bright reflector analysed in Orosei et al.
(2018) at 4 MHz (top) and 5 MHz (bottom).

- 414
- The histograms are asymmetric, with a cut-off at high values and a long tail towards low ones. This characteristic matches the intuitive notion that the intensity of a basal reflection cannot increase indefinitely, and would thus have a maximum possible value obtained when all the factors contributing to decreasing basal echo intensity as discussed above are minimized. Thus, a comparison between simulations and data requires the introduction of a model for the random dispersion of measurements. As it is not possible to quantify separately the importance of each factor contributing to basal echo power attenuation, we derived a model probability density function directly from the data (Fig. 8).
- The long left-sided tails of the histograms in Figure 7 are characteristic of generalized extreme value distributions, often used to model the maxima of sequences of random variables. Although this is a heuristic method

- 424 for the selection of the model distribution, it has the merit of matching data histograms better than other parametric
- 425 distributions.
- 426





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430 Through the remainder of this paper, we use these best-fit distributions as the template for randomly431 generating synthetic measurements from models.

432

## 433 3.5. Electromagnetic propagation model

434

The propagation of radar waves across stratified media is described by non-linear equations dependent on 435 the electromagnetic properties and thickness of the layers, as well as the probing frequency. Here, we model 436 electromagnetic behaviour of stratified CO<sub>2</sub> ice and dust-laden H<sub>2</sub>O ice, by assuming a 1D geometry (Lombardo et al., 437 2000; Pettinelli et al., 2003; Kartashov et al., 2004; Nunes and Phillips, 2006; Courville et al., 2021). Specifically, we 438 439 simulate the propagation of radar pulses through twelve idealized models of the SPLD, consisting of sets of perfectly parallel planar interstratified basal layers composed of CO2 ice and H2O ice, where the latter has variable contents of 440 dust. The total thickness of the simulated deposits was set at the value derived through MARSIS radargrams over the 441 442 study area (1.5 km). The material underlying the deposits was set to be basaltic rock. The simulations were run by code adapted from MATLAB<sup>(TM)</sup> scripts publicly available through a public research data repository (Orosei and 443 444 Cicchetti, 2018). The code computes the complex reflectivity of the layer stack across the range of frequencies within the pulse bandwidth, multiplying it by the signal spectrum and Inverse-Fourier transforming to the time domain. 445 Simulations were run for one, two or three  $CO_2$  ice layers, the lowermost of which is in direct contact with the bedrock, 446 while the remaining ones are separated by layers of H<sub>2</sub>O ice of variable thickness (Fig. 9). CO<sub>2</sub> ice layers are 447



450 Fig. 9. Schematic stratigraphy used in numerical simulations. The model stratigraphy is here shown as a set of planar parallel layers of CO<sub>2</sub> ice (dark blue) and H<sub>2</sub>O ice (light blue), bounded by an upper half space representing the Martian atmosphere (as 451 452 semi-infinite vacuum) and a lower half space representing the Martian bedrock (brown). Simulations are run for one, two or three 453 lossless CO<sub>2</sub> ice layers, the lowermost of which is in direct contact with the bedrock, while the remaining ones are separated by layers of H<sub>2</sub>O ice of variable thickness. The topmost layer of H<sub>2</sub>O ice represents the bulk of the stratigraphy. Layer thicknesses of 454 455 CO2 ice and interlayer dusty water ice range from 0 to up to 100 m, with total deposit thickness = 1.5 km. The red arrow indicates 456 the depth direction (-z). The inverted triangle on top of the sequence indicates the surface of the deposits. The sketch is drawn not 457 to scale. 458

Typically, complex relative dielectric permittivities are strongly dependent on the frequency of the propagating 459 electromagnetic wave and the temperature of the medium. Attenuation of the signal is independent of frequency at 460 461 MARSIS wavelength for pure water ice: we used the empirical formulae reported by Mätzler (1998) for the average surface temperature value of 160 K (Clifford, 1987) taken as a constant across the entire model stratigraphy. We find 462 that the real part of the dielectric permittivity of water ice is 3.11, with loss tangent values between 2.5 10<sup>-8</sup> (3 MHz) 463 and 3.7 10<sup>-8</sup> (5 MHz). The loss tangent of CO<sub>2</sub> ice is not well constrained at the temperature of interest, with 464 extrapolations and upper limits only being reported in the published literature. In our computations therefore, we set it 465 to be = 0, to produce the highest possible subsurface-to-surface echo power ratio values. We did not consider the 466 effect of the complex part of the permittivity of CO<sub>2</sub> on the reflection coefficient, because it is generally assumed to be 467 low ( $\leq 10^{-3}$ ). Computing the Fresnel reflection coefficient at normal incidence for an interface between a layer of CO<sub>2</sub> 468 469 ice and an underlying bedrock with permittivity values such as those used in the simulations, the results, with and without the inclusion of the imaginary part, differ by < 0.00001. 470

471

472 3.6. Simulations

473

474 To calculate the simulated radar waveforms, in our model stratigraphies we assumed perfectly smooth surfaces, an assumption that holds also for small roughness of the illuminated surface, where "small roughness" is 475 defined (Ulaby et al., 1981) by a height <  $\lambda$  /32, which gives a value of 2.35 m at 4MHz. We considered the 476 477 electromagnetic wave transmitted by the radar having a normal incidence with respect to the model stratified structure (ref. to sketch in Fig. 9), and assumed a 1D-model where the only variation of the electromagnetic properties occurs 478 479 along the z-axis (depth). Furthermore, we assumed spatially homogenous layers with a constant complex dielectric permittivity ( $\varepsilon_i$ ) and thickness ( $h_i$ ). The stratified structure is bounded by two half-spaces representative of the 480 atmosphere and the bedrock. This model is the same adopted in previous work (Orosei et al., 2018a; Lauro et al., 481 2019, Lalich et al., 2021a, 2021b). The received signal y(t) is thus computed as: 482

$$y(t) = \mathcal{F}^{-1}[X(f)R(f)], \tag{1}$$

where  $\mathcal{F}^{-1}$  is the inverse Fourier transform, X(f) is the Fourier transform of the signal transmitted by MARSIS antenna, R(f) is the frequency response ( $\Gamma_1(f)$ ) of the layered structure computed from the recursive scattering function  $\Gamma_i(f)$ : 487

$$R(f) = \Gamma_1(f)$$

$$\Gamma_i(f) = \frac{\rho_i + \Gamma_{i+1} e^{-2jk_{i+1}h_{i+1}}}{1 + \rho_i \Gamma_{i+1} e^{-2jk_{i+1}h_{i+1}}},$$
(3)

488

with  $k_i$  the complex-valued wavenumber of the *i*-th layer, and  $\rho_i$  the Fresnel reflection coefficient at the boundary between layer *i*-1 and *i*, given by:

491

$$\rho_i = \frac{\sqrt{\varepsilon_{i-1}} - \sqrt{\varepsilon_i}}{\sqrt{\varepsilon_{i-1}} + \sqrt{\varepsilon_i}},\tag{4}$$

492

The geometry of the problem is modelled as a layered structure, where the upper and lower half space are the same for each simulation, whereas the assumed stratified layer between the atmosphere and the bedrock changes on the basis of the number of  $CO_2$  ice layers, and the thickness of the layers. The ratio between basal and surface power is determined by considering the ratio between the maximum of the square amplitude of y(t) at a time interval containing the echo return from the surface, and that occurring at a time interval containing the echo return from the upper side of the shallower  $CO_2$  ice layer.

Using a multiprocessor machine, we simulated the three  $CO_2$  layer model for every layer thickness between 0 and 50 m at 1-m intervals for three  $CO_2$  layers and two intervening H<sub>2</sub>O layers, for a total of 51<sup>5</sup> simulations. This allowed us to sample completely the parameter space of the models with two- and three-basal  $CO_2$  layers, and thus to locate and explore the properties of local maxima embedded in the three- and five-parameter spaces respectively. We identified local maxima of subsurface to surface power ratio, both at 4 and 5 MHz, and for each of them we extracted the basal echo power ratio for all simulations whose layers are within 2 m of the thickness of those corresponding to the local maximum, thus simulating the effect of random but limited variation of the stratigraphy.

## 507 4. Results

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506

To implement a quantitative comparison between data and simulation results, for each local maximum of subsurface to surface echo power ratio we produced the histogram of power values extracted from its neighbourhood, and convolved it with the template distributions shown in Figure 8, obtaining a simulated histogram which represents the global effect of the factors affecting propagation within the SPLD on model results. An example of a synthetic distribution is shown in Figure 10.



Fig. 10. Comparison between the histogram of measured values of subsurface to surface echo power ratio at 4 (left) and 5 MHz 516 517 (right) with the histogram of model results in the neighbourhood of a given local maximum (see text for details), and with the 518 synthetic histogram of model results produced through the convolution of the histogram of model results with the distribution template shown in Figure 8. The histograms are computed both for model results at 4 and 5 MHz. 519

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521 To make a guantitative comparison of model results with data, the synthetic histograms were used to 522 generate a set of random values representing measurements. This was done by taking each histogram bin, and generating a set of uniformly distributed random numbers in an interval corresponding to the bin, whose quantity is 523 proportional to the bin height. Finally, the set of synthetic measurements was compared to actual measurements 524 through a statistical test to determine if the two sets of samples could be produced by the same distribution. We used 525 the two-sample Kolmogorov-Smirnov test (Kolmogorov, 1933; Smirnov, 1939), which is a nonparametric test for the 526 527 null hypothesis that the data in two sets of samples are from the same continuous distribution. It is widely employed in statistics for its robustness and its sensitivity to both location and shape of distributions. The test was performed using 528 the implementation available in the MATLAB<sup>(TM)</sup> proprietary programming language, and setting the significance level 529 530 for the rejection of the null hypothesis at 5%.

A configuration of layers producing a local maximum at one frequency does not result in a local maximum at 531 the other frequency. For this reason, both local maxima at 4 MHz and at 5 MHz had to be considered. Thus, for a 532 given model (either two- or three-CO2 ice layers) we simultaneously tested samples of model results at 4 and 5 MHz 533 extracted for a set of laver thicknesses corresponding to a local peak of basal echo power at either 4 or 5 MHz, and 534 for all layer thicknesses within two meters of the one producing the peak. This resulted in four possible combinations 535 of number of layers and frequency of the echo power maximum. We found and tested 487 local maxima at 4 MHz and 536 687 at 5 MHz for the two-layer model, and 2981 local maxima at 4 MHz and 5232 at 5 MHz for the three-layer model. 537 Results are shown in Figure 11. 538



539

Fig. 11. Plots of the asymptotic p-values produced by the Kolmogorov-Smirnov test versus the maximum subsurface to surface
 power ratio of simulated echoes, for models with two- and three-CO<sub>2</sub> ice layers and for local maxima at 4 and 5 MHz. Each point
 represents the probability that model results and MARSIS measurements belong to the same continuous distribution. For each
 tested set of simulations, probabilities are computed both at 4 MHz (dots) and at 5 MHz (crosses).

545 No set of two- and three-layer models resulted in simulated values exceeding the 5% significance level 546 threshold. However, it can be seen in the bottom right plot in Figure 11 that a few layer configurations resulting in a 547 local maximum of basal echo power at 5 MHz approach the 5% threshold. This happens only at 5 MHz (crosses in 548 Fig. 11), while at 4 MHz (dots) the probability remains negligible. This quantitatively confirms the observation that, in a 549 model based on the coherent interference between layers, a configuration capable of producing a constructive 550 interference at one frequency is not capable of doing the same at another frequency.

None of the modelled scenarios involving CO<sub>2</sub> ice layers reproduce the distribution of basal echo intensities observed by MARSIS over the bright areas in Ultimi Scopuli. Median values of the simulated basal echo power are lower than those observed in real MARSIS data, and the spread of the simulated values does not match the range of the measured data. We thus conclude that the interpretation that best reconciles all radar observations in Ultimi Scopuli remains that of a strong basal reflector overlain by a thick dust-laden SPLD.

556

## 557 5. Conclusions

558

The results of our simulations do not support claims that CO2 ice layers interbedded with water ice can 559 produce the bright reflections detected by MARSIS from the base of the SPLD in Ultimi Scopuli. Therefore, we rule out 560 the presence of hidden deposits of basal CO<sub>2</sub> ice in this area. Based on these results, and the lack of detection of 561 sequestered CO2 ice deposits elsewhere in the SPLD (Whitten et al., 2017; Whitten and Campbell, 2018; Khuller and 562 Plaut, 2021) beyond those reported by Phillips et al. (2011) and Bierson et al. (2016), we posit that it is unlikely that 563 hidden  $CO_2$  was stored in the late Amazonian (< 250 Ma) south polar deposits. This conclusion is consistent with the 564 geological record of diminishing volcanic activity on Mars during the Hesperian and throughout the Amazonian, with 565 very small amounts of CO<sub>2</sub> released into the atmosphere by volcanic degassing in post-Noachian times. 566

- 567 With the polar caps being the most voluminous reservoir of volatiles on Mars, and their role in regulating the 568 planetary climate, records of the composition and physical properties of the polar layered deposits are fundamental to 569 constrain the entire geological and climatological history of Mars. The ground penetrating radar MARSIS continuing 570 acquisition of observations over the polar regions is an essential element of our investigations into the origin,
- evolution, and inventory of Martian volatiles and of the planet evolution. This is why interpretations of MARSIS data
- 572 must be critically assessed against the framework of the physical theory of the propagation of radar waves through 573 stratified media, as we have demonstrated in this paper. Rigorous application of this approach to all investigations
- 574 based on MARSIS data will advance our knowledge of the nature and properties of Mars's polar materials.
- 575

## 576 Acknowledgments

577

The authors are grateful to A.P. Rossi and L. Guallini for their helpful comments on an earlier version of this manuscript. We thank two anonymous reviewers for their constructive criticism and insights, that contributed to clarify and improve the paper. This work was supported by the Italian Space Agency (ASI) through contract ASI-INAF 2019– 21-HH.0.

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