A New Method to Predict Particle Sizes of Lunar or S-type Asteroid Surfaces Based on The Laboratory Thermal-infrared Data Postprint

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Abstract

The surface particle size and distribution characteristics of celestial bodies (e.g., the Moon, asteroids, etc.) will affect the interpretation of hyperspectral remote sensing data and the implementation of sampling missions. Currently, the estimation of the surface particle sizes is mainly focusing on interpreting the thermal inertia with the infrared spectral data from ground-based or space telescopes, but this method show distinct errors compared with the imaging results of the orbiter. By analyzing some thermal infrared spectral data, a relationship between the particle sizes of the main rock-forming minerals (e.g. pyroxene, feldspar, olivine) and the slopes of their thermal infrared spectrum was found. Based on this relationship, a preliminary model for estimating the grain sizes (30–300 m) of lunar or S-type asteroids' surfaces which are silicate minerals dominated was established, and the correlation coefficients (R2) for most of the rock-forming minerals were better than 90%. Six observational datasets of natural lunar and terrestrial samples are used to validate the model, and the results show a systematical overestimation of the ground-truth particle sizes, the potential causes are analyzed and an additional correction is used to eliminate the overestimation of the particle size prediction. These results are expected to provide guidance for interpretation of lunar and S-type asteroid surface sampling and spectral data.

Full Text

Preamble

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A New Method to Predict Particle Sizes of Lunar or S-type Asteroid Surfaces Based on Laboratory Thermal-infrared Data

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Abstract

The surface particle size and distribution characteristics of celestial bodies such as the Moon and asteroids significantly affect the interpretation of hyperspectral remote sensing data and the implementation of sampling missions. Currently, estimation of surface particle sizes primarily focuses on interpreting thermal inertia using infrared spectral data from ground-based or space telescopes, but this method shows significant errors when compared with imaging results from orbiters. By analyzing thermal infrared spectral data, we identified a relationship between the particle sizes of main rock-forming minerals (e.g., pyroxene, feldspar, olivine) and the slopes of their thermal infrared spectra. Based on this relationship, we established a preliminary model for estimating the grain sizes (30–300 m) of lunar or S-type asteroid surfaces dominated by silicate minerals, achieving correlation coefficients (R^2) better than 90% for most rock-forming minerals. Six observational datasets of natural lunar and terrestrial samples were used to validate the model. The results show systematic overestimation of ground-truth particle sizes; potential causes were analyzed and an additional correction was applied to eliminate this overestimation. These results are expected to provide guidance for interpreting lunar and S-type asteroid surface sampling and spectral data.

Key words: infrared: planetary systems – minor planets, asteroids: general – techniques: imaging spectroscopy

1. Introduction

The surface particle size and distribution characteristics of celestial bodies such as the Moon and asteroids play an important role in surface landing, roving, and sampling operations. The surfaces of celestial bodies are covered with a thick layer of loose dust, which is unfavorable for landing probes and rover maneuvering due to its low load-bearing capacity (Yue et al. 2020). Furthermore, particle size plays a pivotal role in the identification and quantification of material composition through visible and near-infrared (VIS-NIR) spectroscopy (Poulet et al. 2007; Ody et al. 2013) and thermal infrared (TIR) spectroscopy (Logan & Hunt 1970; Hunt & Logan 1972; Logan et al. 1973; Mustard & Hays 1997; Shirley & Glotch 2019).

For example, the 1 m absorption position and width of olivine are strongly affected by particle size and become difficult to recognize (Poulet et al. 2007). Previous studies have also shown that particle size significantly impacts thermal infrared spectral Reststrahlen bands (RBs) and transparency features (TFs) (Lyon 1962), causing changes in spectral contrast as well as shifts in positions of Christiansen features (CFs), RBs, and TFs (Logan & Hunt 1970; Shirley & Glotch 2019). Information regarding particle sizes on the surfaces of celestial bodies can also facilitate deeper comprehension of geological environments, surface-related processes, and the formation and evolution of these bodies (Noble et al. 2001; Hamilton et al. 2021).

Currently, the mainstream method for predicting particle size on celestial body surfaces involves detecting and determining thermal inertia (Kieffer et al. 1973; Presley & Christensen 1997). Thermal inertia measures how strongly surface materials resist temperature change under varying solar insolation conditions and is strongly affected by regolith particle size, porosity, and composition. Therefore, it has been used as an indicator of particle size for celestial bodies (Emery et al. 2006; Okada et al. 2020; Cambioni et al. 2021). However, due to uncertainties in thermal inertia modeling involving various physical parameters (Presley & Christensen 2010; Gundlach & Blum 2013), this approach has limitations. According to imaging results from the U.S. OSIRIS-REx mission, the surface of C-type asteroid Bennu is composed mainly of boulders larger than 1 m in diameter (DellaGiustina et al. 2019), contradicting predictions of a surface dominated by 0.5–5 cm particles derived from thermal inertia data from OTES. The particle sizes on Bennu's surface exceeded the design specifications of the OSIRIS-REx spacecraft and posed significant challenges for sampling (Lauretta et al. 2019).

TIR spectroscopy has played an important role in particle size prediction and composition identification on celestial body surfaces. Silicate minerals are the main constituents of rocky celestial bodies. The presence of RB, CF, and TF features in the TIR spectral range is closely related to silicate composition and can be used as an indicator to discriminate their composition. The CF is generally considered to be caused by rapid changes in the refractive index (i.e., anomalous dispersion) of a single molecule prior to its fundamental vibrational band, which is close to that of the refractive index of the surrounding medium, minimizing backward scattering. Characterized spectroscopically as a reflectance minimum or emissivity maximum, CF can be used as a diagnostic indicator for minerals even when RB is attenuated (Conel 1969). The RB is caused by stretching of the Si-O bonds in silicate minerals and is related to the mineral's composition.

The TF exists in the volume scattering region between Si-O stretching and bending fundamental vibration bands and is characterized as emissivity minima or reflectivity maxima (Salisbury et al. 1991). Shirley & Glotch (2019) detailed the effect of particle size on TIR spectra under simulated lunar environment conditions, demonstrating that the spectral contrast of RBs and TFs is enhanced as particle size decreases, and that CF positions shift to longer wavelengths as particle size decreases (Logan & Hunt 1970; Hunt & Logan 1972; Logan et al. 1973; Mustard & Hays 1997; Shirley & Glotch 2019).

TIR spectrometers have been employed in many space exploration missions. As early as the 1990s, Mariners 6, 7, and 9 carried TIR spectrometers (Hanel et al. 1972a, 1972b; Conrath et al. 1973; Pimentel et al. 1974), providing pioneering information on the composition and properties of the Martian surface and atmosphere. The OSIRIS-REx Thermal Emission Spectrometer (OTES) remotely detected mineral and thermophysical properties of C-type asteroid Bennu (Hamilton et al. 2021). China will launch its first asteroid exploration and sample return mission in 2025. As one of the scientific payloads, the Asteroid Thermal Emission Spectrometer (ATES) will perform TIR spectroscopic surveys on the surface of near-Earth S-type asteroid 2016 HO3 at different altitudes and local times (Zhang et al. 2021). Based on the requirements of this first asteroid sampling mission and the uncertainties in particle size prediction, we developed a new method to predict particle sizes based on TIR spectroscopy. For the same mineral, the slopes of the spectrum near the longer wavenumber side of the CF increase with decreasing particle size (Logan & Hunt 1970; Hunt & Logan 1972; Logan et al. 1973; Mustard & Hays 1997; Shirley & Glotch 2019). According to this relationship, we can derive particle size information by calculating spectral slopes near the longer wavenumber side of the CF. This method is expected to be useful for future remote sensing and sampling of lunar or S-type asteroid surfaces dominated by silicate minerals.

2. Samples and Data Description

The asteroid 2016 HO3 is thought to be an S-type asteroid with a silicate-dominated composition (Sharkey et al. 2021). Therefore, this study prepared samples of three common silicate minerals (olivine, pyroxene, and feldspar) and their mixtures (Table 1). Each sample was ground into seven distinct particle sizes. Additionally, three groups of mixed samples with varying particle sizes and mass ratios of pyroxene and labradorite were prepared as simplified analogs of gabbro: (1) a mixture of 10wt% augite and 90wt% labradorite, (2) a mixture of 30wt% augite and 70wt% labradorite, and (3) a mixture of 50wt% augite and 50wt% labradorite.

We note that the average grain size of lunar soils is 60 m, and grain size is also related to depth, with material at the top of the space-weathered layer exhibiting smaller average grain sizes (King et al. 1971; King et al. 1972; McKay et al. 1972, 1974; Carrier 1973; Heiken et al. 1973). Opportunity's exploration of Meridiani Planum on Mars revealed a dark weathering layer near the landing site approximately 1 m thick with grain sizes no larger than 125 m (J. Q. Li et al. 2016). Shirley & Glotch (2019) investigated the effect of particle size on TIR spectral features of different minerals in a simulated lunar environment using seven particle size ranges: <32 m, 32–63 m, 63–90 m, 90–125 m, 125–250 m, and >250 m. However, there remains a lack of data for larger particle sizes, particularly in the 250–450 m range. We therefore ground and wet-sieved all samples to seven different particle sizes with a wider range (30–450 m): 30–54 m, 54–76 m, 76–100 m, 100–150 m, 150–200 m, 200–300 m, and 300–450 m. Due to humid summer weather, two mixture samples with particle sizes of 30–54 m and 54–76 m experienced agglomeration prior to spectral measurement. We dried these mixture samples in an oven at 60°C for more than 24 hours before spectral testing to ensure accuracy.

The process for acquiring TIR emissivity spectral data was as follows: Samples were poured into aluminum cups with a diameter of 3 cm to maintain a rough surface similar to natural regolith. Spectral measurements were carried out using a Bruker 80v Fourier Transform Infrared (FTIR) spectrometer, and reflectance data were first collected using an integrating sphere accessory. The infrared beam enters the integrating sphere and illuminates a deflector mirror mounted inside the sphere, which directs the beam to the lower sample port and illuminates the samples at an incidence angle of 13°. The reflected and scattered light inside the sphere is then collected by a detector located behind the exit port to obtain reflectance data (R). The integrating sphere is gold-plated with a gold plate serving as the calibration target.

Since the powder samples are thick enough to neglect transmission, the measured reflectance (R) can be converted to emissivity (E) according to Kirchhoff's law of thermal radiation (E = 1 - R). Each sample's spectrum was acquired over the range of 4000–400 cm^{-1} at ambient temperature and pressure using 128 scans with a resolution of 8 cm^{-1} and a total scanning time of 5 minutes. The spectrum was then normalized by setting the maximum emissivity value to 1. The position of the CF for each sample was obtained by fitting the maximum emissivity (Donaldson Hanna et al. 2012).

3. Prediction Method for Particle Size

We plotted all TIR emissivity spectra of samples with different particle sizes (Figure 1). From Figure 1, we identified a relationship between particle size and spectral slopes: for the same sample, spectral slopes on the longer wavenumber side of the CF gradually become steeper with decreasing particle size. Based on this relationship, we developed a new method to predict particle sizes by calculating spectral slopes near the longer wavenumber side of the CF. This requires determining the emissivities and corresponding wavenumbers at two data points.

One data point is undoubtedly the position of the CF and its corresponding emissivity value. According to TIR spectral characteristics of different minerals, we find that there is usually a steep increase in emissivity between wavenumbers of 2250–1333 cm^{-1} and 1176–870 cm^{-1} as wavenumbers decrease. The 2250–1333 cm^{-1} region is dominated by volume scattering, while the 1176–870 cm^{-1} region is dominated by surface scattering and RBs. This sharp increase in emissivity marks the transition from volume to surface scattering and is referred to by Doug Nash as the "transition edge," which clearly indicates the CF feature position (Salisbury et al. 1991). To determine the CF position for each mineral, we defined it by fitting a second-order polynomial to the emissivity maxima of each mineral spectrum following Donaldson Hanna et al. (2012). The CF position is generally located in the wavenumber range of 1100–1400 cm^{-1}. If more than one emissivity maximum appears in the spectrum, we followed Salisbury & Walter (1989) and Cooper et al. (2002) in selecting the emissivity maximum at the longest wavenumbers to fit the CF position.

The other data point should be selected in the wavenumber range of 1700–1400 cm^{-1}, which is dominated by volume scattering. Typical particulates of igneous rocks on planetary surfaces often contain hydrated or hydroxylated minerals that exhibit an H-O-H bending vibration feature near 1613 cm^{-1} (Salisbury & Walter 1989). For olivine and pyroxene, there are also prominent features at 1333.3 cm^{-1} caused by absorption from overtone and combination tone vibrations (Salisbury et al. 1991). To avoid these spectral features, we selected a wavenumber of 1500 cm^{-1} and its corresponding emissivity value as the second data point for spectral slope calculation. The equation for calculating spectral slope is defined as:

$$K = \frac{\varepsilon_{CF} - \varepsilon_{1500}}{\omega_{CF} - 1500}$$

where K represents the slope between 1500 cm^{-1} and the CF position, _{CF} is the emissivity at the CF position, _{1500} is the emissivity at 1500 cm^{-1}, and ω_{CF} is the wavenumber of the CF position.

4.1. Particle Size Estimation Model

Following the method described in Section 3, we first calculated the CF positions of all samples (Table 2). The CF positions of olivine vary between 1114 and 1130 cm^{-1} as grain size changes, with a mean value of 1122 cm^{-1}. The CF positions of mixed sample 1 (90wt% labradorite) fluctuate between 1249 and 1281 cm^{-1}, with a mean value of 1268 cm^{-1}. The CF positions of mixed sample 2 (70wt% labradorite) fluctuate between 1238 and 1281 cm^{-1}, with a mean value of 1258 cm^{-1}, while the CF positions of mixed sample 3 (50wt% labradorite) fluctuate between 1238 and 1249 cm^{-1}, with a mean value of 1249 cm^{-1}. The CF positions in mixed samples move toward shorter wavenumbers as labradorite content decreases, whereas minerals with higher magnesium-iron content, such as olivine, have even shorter wavenumbers at the CF position, consistent with previous observations (Logan & Hunt 1970; Shirley & Glotch 2019).

After calculating CF positions for all samples, we derived spectral slopes (K-values) using Equation (1). As shown in Table 3, the calculated K-values are consistent with observed patterns, with the absolute value of spectral slope increasing as particle size decreases.

We further used exponential function fitting to explore the relationship between K-values and grain sizes (Figure 2). Results show that K-values initially increase with particle size, reach maximum values when particle sizes increase to 300 m, and then tend to stabilize with further particle size increases. The exponential function is modeled as $y = a\,exp(bx) + c$, where the fitting coefficients a, b, c and correlation coefficient (R^2) are listed in Table 4. The results demonstrate that exponential function fits achieve $R^2 > 0.90$ for all samples, with olivine showing the best fit.

It should be noted that each particle size range has a width, and we employed the mean grain size when plotting the relationship between K-values and particle sizes. For example, for the range of 54–76 m, 65 m was used as the horizontal coordinate value.

As illustrated in Figure 1, spectral curves on the longer wavenumber side for particle sizes of 200–300 m and 300–450 m overlap, making their K-values indistinguishable. There are even cases where K-values for larger particle sizes are smaller than those for smaller sizes, contrary to the observed pattern. For example, the K-value for mixture 1 with particle size 300–450 m is less than that for the 200–300 m case. We therefore speculate that our proposed method may not be applicable for grain sizes exceeding 300 m.

From Figure 2, the fitted curves and their corresponding coefficients for the three mixture groups demonstrate striking similarity. With increasing mafic component content (e.g., pyroxene), the curves become progressively flattened (reduced curvature). Notably, the curve for olivine is even more flattened, indicating that enhanced mafic components correlate with gradual flattening of fitted curves, consistent with observed CF position shifts toward longer wavelengths at higher mafic concentrations.

4.2. Effects of Moisture

Mixture samples in both the 30–45 m and 45–76 m particle size classes experienced agglomeration due to wet weather, with the 30–45 m size class showing more serious agglomeration, resulting in effective particle sizes larger than the 45–76 m class. To ensure measurement accuracy and avoid moisture effects, we dried the two mixture samples at 60°C for more than 24 hours. Oscillation was also applied after drying to further disperse agglomerates.

TIR spectral measurements were conducted on both mixture sample classes before and after drying (Figure 3). As illustrated in Figure 3, TIR spectra of the three mixture groups within the 54–76 m particle size range exhibit minimal variation before and after drying, indicating no moisture-induced agglomeration occurred. In contrast, emissivity on the longer wavenumber side of the CF for the three mixture groups in the 30–45 m particle size range decreased significantly after drying, and spectral slopes became steeper, suggesting that moisture agglomeration was substantially mitigated by drying.

4.3. Physical Mechanism Discussion

We have established the relationship between thermal spectral slope and particle size: as particle size decreases, the absolute value of the spectral slope on the longer wavenumber side of the CF feature increases. This phenomenon may be explained as follows: volume scattering dominates for all particle sizes in wavenumber regions close to the CF feature. As particle size gradually decreases, sample particles transition from optically thick to thin, and the degree of volume scattering increases, leading to lower emissivity or higher reflectivity and ultimately greater spectral contrast on the longer wavenumber side of the CF (Cooper et al. 2002). In weak absorption regions of the TIR range, spectral contrast increases with decreasing particle size due to increased volume scattering (Bishop et al. 2019). Therefore, as particle size becomes larger, spectral contrast decreases and spectral slope K-values converge slowly toward zero, a trend that aligns with the intrinsic convergence behavior of exponential functions.

This result also explains why K-values for mixture samples with 200–300 m and 300–450 m particle sizes are not well differentiated.

4.4. Model Validation and Limitation Discussion

We selected TIR spectra of four typical samples from the RELAB spectral library to validate our particle size prediction model. Typical samples included lunar olivine, mare basalt, and two terrestrial gabbros. To better approximate test data from celestial regolith surfaces, we additionally selected two Apollo lunar soil spectral datasets (data source: Morlok et al. 2022). Particle size characteristics and sample descriptions are detailed in Table 5. Apollo lunar soil spectral data include modal mineralogy estimates (Table 6).

Following Kirchhoff's law (E = 1-R), reflectance data were converted to emissivity spectra (Figure 4). These emissivity data were normalized using the methodology described in Section 2, with subsequent CF position calculations (Table 7). Figure 4 reveals a consistent trend across lunar and terrestrial samples: finer particle sizes correlate with increasingly steep spectral slopes on the long-wavenumber side of the CF.

We calculated spectral slope K for all test samples (Table 7) and subsequently predicted particle sizes using our model, with results visualized in Figure 5. Notably, predictions for specimens AN-G1M-011-C (200–500 m) and AN-G1M-011-D (500–2000 m) were excluded from Figure 5 as they exceeded the model's applicable particle size range, as evidenced by their anomalously elevated predictions.

Figure 5 demonstrates that predicted particle sizes for two Apollo lunar soil groups match measured values better than other samples, though most predictions remain systematically higher. This discrepancy may stem from two factors.

First, the analog samples used in our modeling are common silicate minerals ground to single-mineral grains or mixtures of single-mineral grains. However, actual lunar or S-type asteroid regolith compositions are more complex. Studies on Chang'e-5 returned samples indicate that lunar regolith typically consists of multi-mineral aggregates, basaltic fragments, breccia components, glass, and agglutinates (Cao et al. 2025). The freshly ground samples used in our model have brighter surfaces, whereas natural terrestrial and lunar samples used for validation are multi-mineral aggregates that experience weathering effects that darken surfaces and reduce reflectance (Nimura et al. 2008; Wang et al. 2017; Shirley 2018). This weathering particularly diminishes spectral contrast between near-infrared and mid-infrared regions (Yang et al. 2022), leading to higher emissivity values in our study. Consequently, emissivity at 1500 cm^{-1} (_{1500}) exceeds modeled values, increasing the K-value. This is likely the primary factor affecting model accuracy.

Second, CF position variations contribute to the discrepancy. Comparative spectral analyses between model and test samples (e.g., lunar versus terrestrial olivine in Figure 6, augite-labradorite mixtures versus rock spectra in Figure 7) show that test samples exhibit CF positions either matching or shifted toward lower wavenumbers, which leads to a slight increase in the K-value for iron-enriched, magnesium-depleted compositions. CF positions intrinsically depend on mineral composition, with natural samples displaying greater complexity due to heterogeneous mineral proportions (Cooper et al. 2002; Salisbury et al. 1991). Even within mineral groups, CF positions shift with chemical composition. Lunar olivines in Figure 6 exhibit CF positions shifted toward longer wavelengths compared to terrestrial counterparts, attributable to their higher Fe/(Fe+Mg) ratios. Laboratory studies show that higher forsterite content shifts CF positions to higher wavenumbers (Hamilton 2010; Lane et al. 2011), consistent with lunar olivine composition (Yang et al. 2022). Based on CF position ranges for pyroxene and feldspar (two main constituents of lunar and S-type asteroids), we estimate that CF positions of lunar and S-type asteroids could only be located in the wavenumber range of 1180–1288 cm^{-1}, and particle size prediction errors induced by CF position variations could be less than 20%.

The combined effects of weathering and CF position shifts synergistically elevate K-values, ultimately resulting in systematic overestimation of particle sizes. To enhance model reliability and practical application, we fitted predicted particle size values against ground truth and derived a correction formula to eliminate this systematic bias (Figure 5). The formula is $y = 0.79x - 17.5$, where x denotes values predicted by the particle size estimation model and y represents corrected values. The calibrated model demonstrates optimal predictive performance for silicate-dominated regolith surfaces with particle sizes ranging from 30–300 m.

Most extraterrestrial rock fragments may also contain other minerals such as sulfides, phosphates, or glass phases. Glass phases may constitute a significant proportion of lunar regolith and cause "broad and smooth" morphologies in RB features of reflectance spectra, but they likely do not affect diagnostic CF positions (Nash & Salisbury 1990; see Figure 2 in Morlok et al. 2022). Similarly, some phosphate minerals exhibit distinct spectral features in the 1200–900 cm^{-1} range due to P-O stretching vibrations (Lane et al. 2011b), but their low abundance in lunar regolith means spectral characteristics remain dominated by silicate minerals (see Figure 2 in Morlok et al. 2022). Sulfides only show significant spectral features below 450 cm^{-1} (Bishop et al. 2019), thus their influence on the particle size estimation model is negligible.

Although our intimate mixtures of binary mineral particles (augite-labradorite) cannot fully replicate the spectral characteristics of actual regolith surfaces with complex mineralogical scenarios, these synthetic mixtures allow controlled isolation of specific physical properties—particularly the relative proportions of mafic versus felsic components—to systematically evaluate their impacts on CF positions. This approach facilitates quantitative assessment of factors driving spectral variations. Furthermore, spectra from simple binary mixtures of augite and labradorite provide meaningful analogs for immature lunar regolith particles (Crown & Pieters 1987).

Our particle size estimation model currently demonstrates optimal applicability under two specific scenarios: (1) silicate-dominated surfaces with substantial pyroxene-feldspar assemblages (higher pyroxene-feldspar abundances correlate with enhanced model performance), and (2) regolith-covered terrains where particle sizes fall below 300 m. The model is inapplicable to bare bedrock boulders.

5. Summary and Future Work

Laboratory studies have demonstrated that mineral particle size significantly affects TIR spectra, which in turn influences the ability to identify and interpret surface composition of celestial bodies. Particle size is also an important factor for mission planning, including landing site selection and sampling. However, methods for predicting particle sizes on target object surfaces are currently scarce and imperfect. In this study, analysis of TIR spectral data from terrestrial minerals and mixtures revealed a correlation between particle size and TIR spectral slopes. Based on this relationship, we established a new model for predicting particle sizes of minerals and mixtures, providing a novel approach for predicting particle sizes on celestial body surfaces.

Our new method predicts particle sizes by analyzing particle size influence on TIR spectra. However, TIR spectral characteristics are also affected by many other factors, particularly the presence or absence of atmosphere. Previous experiments have demonstrated that spectral contrast of RBs and TFs is enhanced and CF feature positions shift to longer wavelengths as particle size decreases on airless body surfaces (Logan & Hunt 1970; Shirley & Glotch 2019). Other influencing factors include porosity (Logan et al. 1973; Salisbury & Eastes 1985), surface roughness (Bandfield 2009; Bandfield et al. 2015; Davidsson et al. 2015), and space weathering (Hapke et al. 1975; Glotch et al. 2015; Lucey et al. 2017). These factors are not currently considered in our particle size prediction model and require further investigation. Nevertheless, our study provides a new idea and useful attempt for predicting particle sizes on silicate-dominated celestial surfaces.

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Note: Figure translations are in progress. See original paper for figures.

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