Correcting for systematic error and quantifying uncertainty on alpha-ejection corrections and eU in apatite (U-Th)/He chronology based on crystal shape and size

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1. Can we correct for systematic error and quantify uncertainties on Ft, Rs, and volumes (concentrations) for commonly analyzed grains?

- We build upon previous work [1-4] and propose rule of thumb corrections and uncertainties for Ft, volume (concentration), and Rs based on realistic grain geometries and populations.
- The correction for systematic error was minimized as much as possible by optimizing measurement parameters.
- Applying these corrections and uncertainties can fit seamlessly into existing lab workflows (ie. do not require extra equipment or complicated procedures).
- Ft uncertainties can be propagated into the uncertainty on the corrected (U-Th)/He date.
- Volume (concentration) uncertainties can be propagated into the uncertainty on eU concentration.

What is geometric uncertainty?

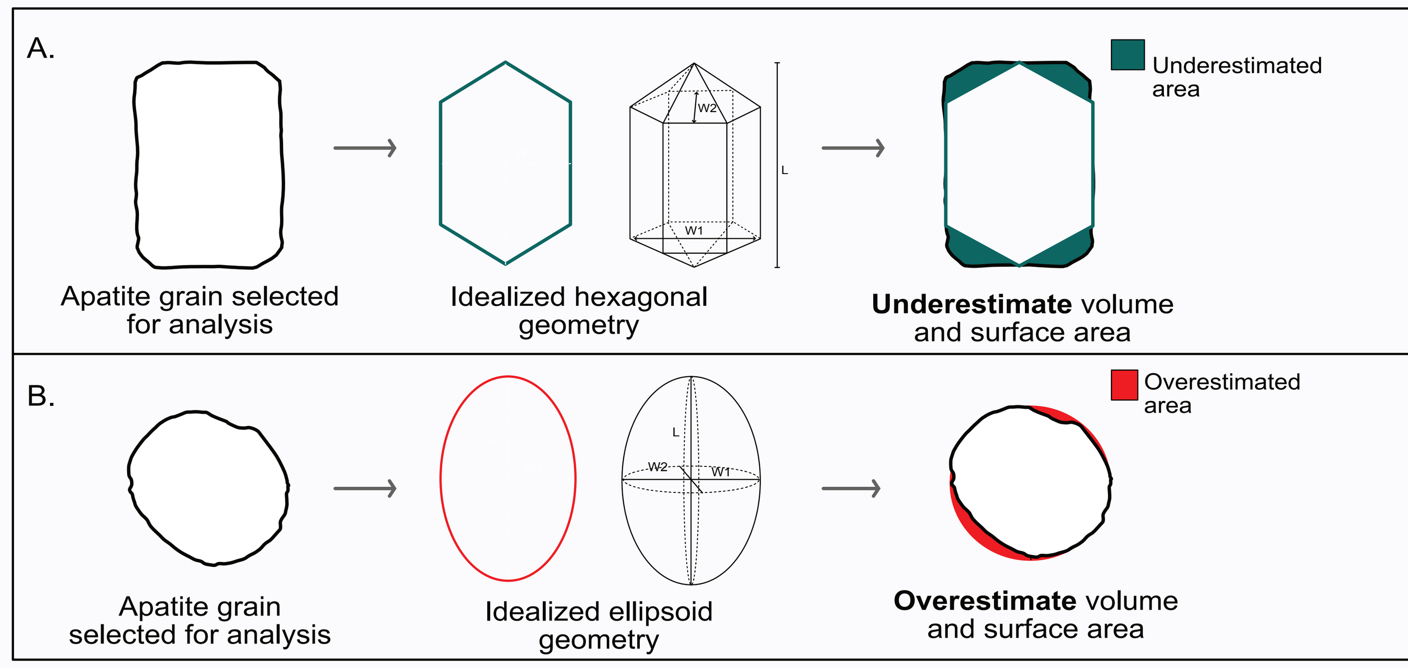


Figure 1.
A. Using an idealized hexagonal geometry [5] to calculate volume, surface area, and subsequent parameters leads to the area in green being excluded.
B. Using an idealized ellipsoid geometry [5] has the opposite effect and leads to the areas in red being overestimated. This effect increases with increasing grain roughness.

* Geometric uncertainty does not include uncertainty from breakage, abrasion, or zonation.

2. Methods

1. Surveyed hundreds of grains to construct GEM (Figure 2) and gained a sense of the range of grain characteristics.

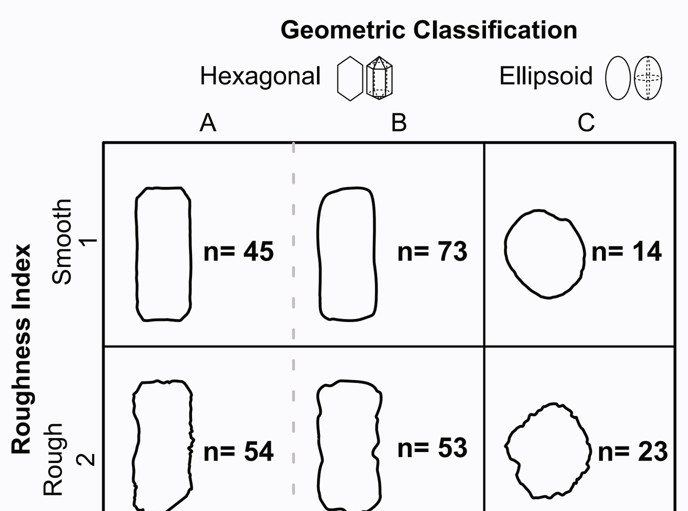


Figure 2. Grain Evaluation Matrix (GEM). A, B, C describe geometry from hexagonal to ellipsoid. 1, 2 describe roughness from smooth to rough. This allows one term, eg. B1, to describe a grain. Numbers in each box are the number of grains of that morphology in our population. N = 262.

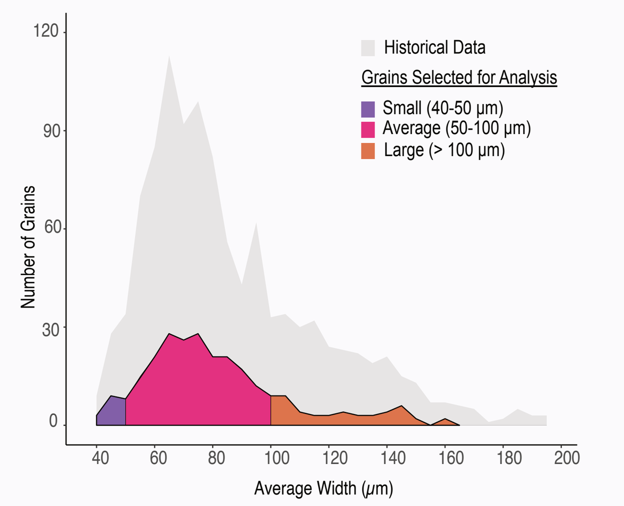
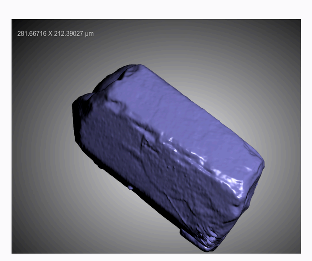


Figure 3. The distribution of grain sizes we analyzed closely matches the historical record of 1100 apatite grains run in the TRaIL 2017-2019.

2. Selected a **representative population** of 262 apatite and measured them in 2D and 3D.
   - Samples: 5 intrusive, 1 extrusive, 2 detrital
   - Age range: Oligocene - Archean
   - Size distribution: 40-170 μm (Figure 3)
   - Morphological distribution: Figure 2



3. Acquired 2D measurements via photomicrograph and calculated volume, Ft, Rs ($Rs = Rs_{Ft}$ [4]) using the equations of Ketcham et al., 2011 [5] for hexagonal and ellipsoid geometries.

4. Used nano-computed tomography (nano-CT) to obtain 3D models of each grain and acquired values for volume, Ft, and Rs from 3D data using Blob3D [6].

3. Corrections for systematic error were determined via bootstrap regression:

- Bootstrapped slopes were generated for each grain geometry using weighted least squares linear regression.
- Intercepts are fixed at 0 for simplicity. Each geometry's slope includes 0 in its 90% confidence interval.
- Corrections are the mean of the bootstrapped slopes.
- A and B grain geometries were combined into a single group (hexagonal), while C is distinct (ellipsoid).

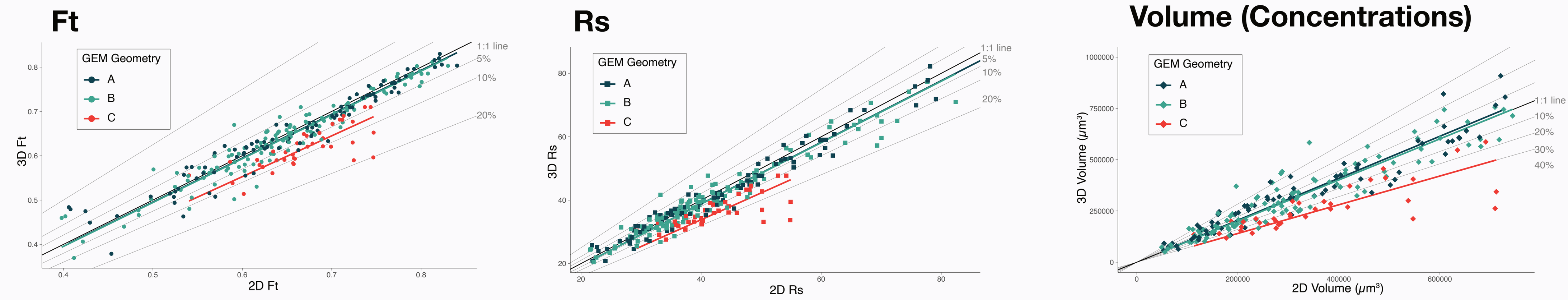


Figure 4. 2D measurements vs. 3D measurements. Note how for all parameters, A and B geometries overlap, while C geometries are distinct. The colored lines are the regression, while the dotted lines are percent deviation from the black 1:1 line.

4. Uncertainty (1σ) on the corrected value was determined using the standard deviation of the residuals:

- Uncertainty on the corrected Ft and Rs value is controlled primarily by grain size.
- Uncertainty on the corrected volume (concentration) value is controlled primarily by grain roughness.

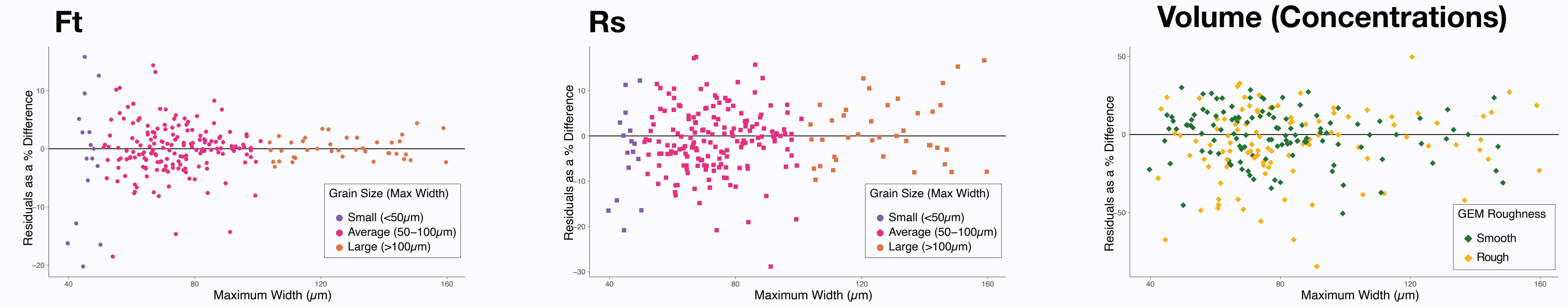


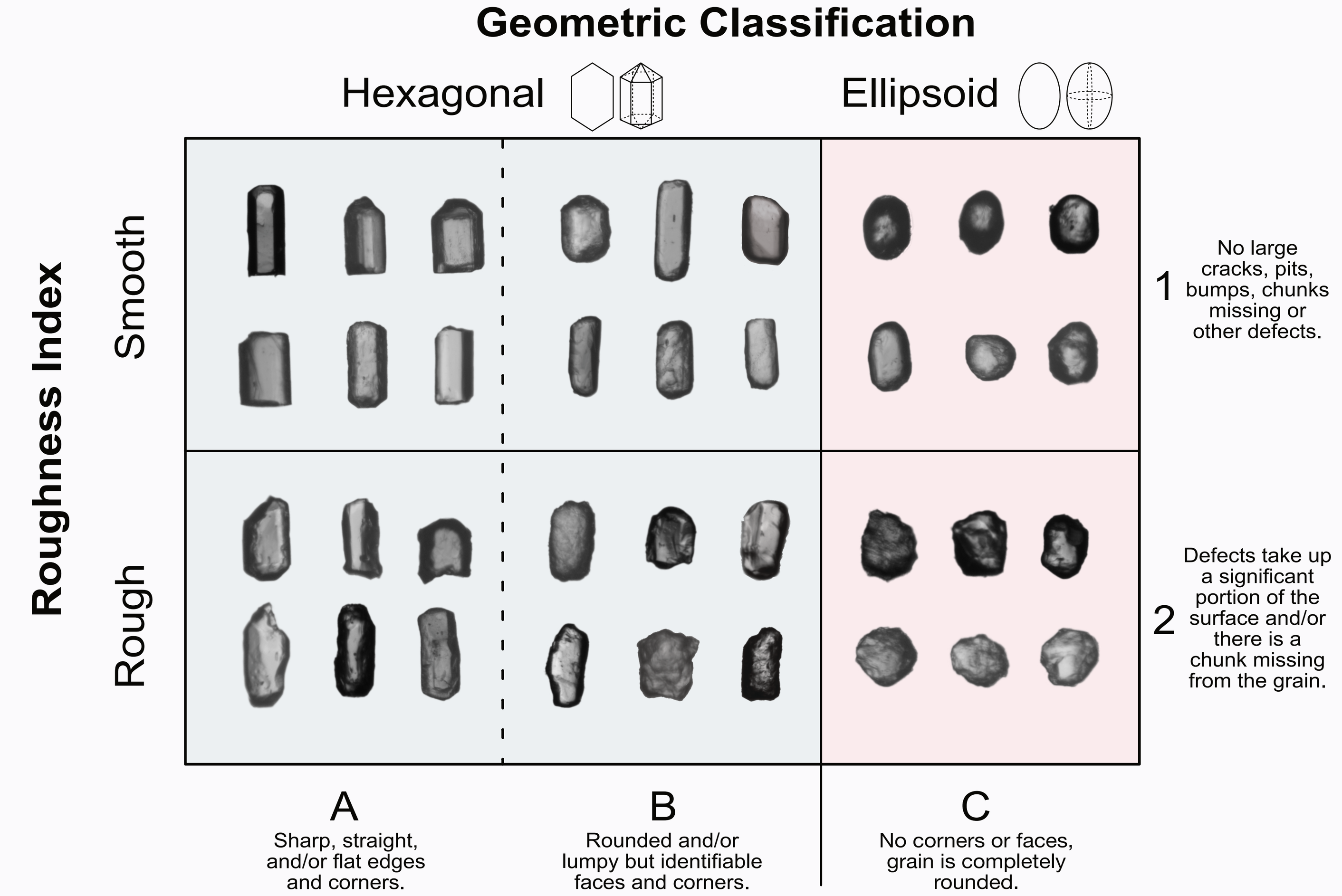
Figure 5. Residuals as a percent difference vs. maximum width. The standard deviation (SD) of Ft residuals are controlled by size. As size increases, SD decreases. Rs-Ft residuals show a weaker correlation with size, but the trend remains. The SD of volume residuals are controlled by roughness. As grain roughness increases, SD increases. See Figure 1.

5. Conclusions: corrections and uncertainties

The Grain Evaluation Matrix (GEM):

Why is the GEM useful?

- It is a tool for simple, effective, and reproducible grain description.
- The GEM axes (geometry and roughness) influence the corrections for systematic error and uncertainties.



Geometric uncertainty (1σ) ranges between 2% and 10% for corrected Ft and 16-24% for corrected volumes (concentrations):

How to use:

1. Calculate 2D values
Calculate Ft, Rs, and volume using the equations of Ketcham et al., 2011 and the maximum width.

2. Apply correction
Based on *grain geometry*, choose and apply the proper corrections.

3. Apply uncertainty
Choose and apply the proper uncertainty to the corrected value.
- Ft and Rs: uncertainty is based on *size*
- Volume (concentrations): uncertainty is based on *roughness*

4. Propagate uncertainty
- Propagate Ft uncertainty into the uncertainty on the corrected (U-Th)/He date.
- Propagate the volume (concentration) uncertainty into the uncertainty on eU.

Ft Corrections: (Uncertainty is controlled by **size**)

Size Index	Hexagonal (A, B)	Ellipsoid (C)
Large (Max Width > 100 μm)	Ft_{corr} **± 2%** = Ft_{2D} x 1.01	Ft_{corr} **± 5%** = Ft_{2D} x 1.10
Average (Max Width 50-100 μm)	Ft_{corr} **± 4%** = Ft_{2D} x 1.01	
Small (Max Width <50 μm)	Ft_{corr} **± 10%** = Ft_{2D} x 1.01	

Rs Corrections: (Uncertainty is controlled by **size**)

Size Index	Hexagonal (A, B)	Ellipsoid (C)
Large (Max Width > 100 μm)	Rs_{corr} **± 7%** = Rs_{2D} x 1.03	Rs_{corr} **± 10%** = Rs_{2D} x 1.17
Average (Max Width 50-100 μm)	Rs_{corr} **± 7%** = Rs_{2D} x 1.03	
Small (Max Width <50 μm)	Rs_{corr} **± 10%** = Rs_{2D} x 1.03	

Volume (concentration) Corrections: (Uncertainty is controlled by **roughness**)

Roughness Index	Hexagonal (A, B)	Ellipsoid (C)
Smooth 1	V_{corr} **± 16%** = V_{2D} x 0.98	V_{corr} **± 22%** = V_{2D} x 1.34
Rough 2	V_{corr} **± 24%** = V_{2D} x 0.98	

A: Sharp, straight, and/or flat edges and corners. B: Rounded and/or lumpy but identifiable faces and corners. C: No corners or faces, grain is completely rounded.

NOTE: These corrections and uncertainties assume maximum width measured perpendicular to the C-axis. We assume ejection occurs through every surface. All Ft-corrections use ^{238}U-Ft.

Citations: [1] Herman et al., 2007. 10.1016/j.chemgeo.2007.03.009 [2] Evans et al., 2008. 10.1016/j.chemgeo.2007.03.009 [3] Glotzbach et al., 2019. 10.1016/j.chemgeo.2018.12.032 [4] Cooperdock et al., 2019. 10.5194/gchron-1-17-2019. [5] Ketcham et al., 2011. 10.1016/j.gca.2011.10.011 [6] Ketcham, R.A., 2005.10.1130/GES00001.1

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