Comparing predicted and observed spatial boundaries of geologic phenomena: Automated Proximity and Conformity Analysis applied to ice sheet reconstructions

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Abstract

Comparing predicted with observed geologic data is a central element of many aspects of research in the geosciences, e.g., comparing numerical ice sheet models with geomorphic data to test ice sheet model parameters and accuracy. However, the ability to verify predictions using empirical data has been limited by the lack of objective techniques that provide systematic comparison and statistical assessment of the goodness of correspondence between predictions of spatial and temporal patterns of geologic phenomena and the field evidence. Much of this problem arises from the inability to quantify the level of agreement between straight or curvilinear features, such as between the modeled extent of some geologic phenomenon and the field evidence for the extent of the phenomenon. Automated Proximity and Conformity Analysis (APCA) addresses this challenge using a system of Geographic Information System-based buffering that determines the general proximity and parallel conformity between linear features. APCA results indicate which modeled output fits empirical data, based on the distance and angle between features. As a result, various model outputs can be sorted according to overall level of agreement by comparison with one or multiple features from field evidence, based on proximity and conformity values. In an example application drawn from glacial geomorphology, APCA is integrated into an overall model verification process that includes matching modeled ice sheets to known marginal positions and ice flow directions, among other parameters. APCA is not limited to ice sheet or glacier models, but can be applied to many geoscience areas where the extent or geometry of modeled results need to be compared against field observations, such as debris flows, tsunami run-out, lava flows, or flood extents.

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1. Introduction

Comparing predicted patterns against field observations is a necessity within many of the geosciences, but most attempts to accomplish this are qualitative or relative. For example, debris flow run-outs are frequently simulated and compared to field observations (Rickenmann and Kock, 1997; Ghilardi et al., 2001; Laigle et al., 2003; Lo and Chau, 2003), but this is generally accomplished using simple, visual comparisons reported as a “reasonable fit”. Accurate simulations of the geometry of a debris fan may assist efforts to
delineate various hazard zones or to distribute appropriate land use permits for areas susceptible to potential debris flows (Aleotti and Polloni, 2003). The results of manual and computer-based methods for delineating watersheds have been compared using percentages of area overlap between models, but this method was unable to assess and report the geometry or conformity between predicted and observed spatial boundaries (Stanton, 2001). Other fields within the geosciences, such as modeling or reconstructing tsunami run-outs (Imamura et al., 1994; Dawson et al., 1996; Downes and Stirling, 2001) or various configurations of flood extent (Mann et al., 1999; Fisher et al., 2002; Teller et al., 2002; Clarke et al., 2004), and even estimating the location of paleo-shorelines (Leverington et al., 2002), are confronted with identical predicaments and generally end up with comparisons of the geometry or extent of various models based on qualitative approaches.

The approach to addressing the problem of comparing model results with field data presented in this paper was driven by work combining glaciological models with geomorphologic field evidence. Understanding the spatial and temporal dynamics of paleo-ice sheets is critical to global climate models and is a core research area in glaciology and glacial geomorphology. Two methods are generally used to reconstruct paleo-ice sheets: (a) numerical ice sheet modeling (Andrews and Mahaffy, 1976; Denton and Hughes, 1981; Hindmarsh et al., 1989; Huybrechts and T'siobbel, 1995; Hughes, 1998), and (b) geologic and geomorphic reconstructions (Boulton et al., 1985, 2001; Dyke and Prest, 1987; Kleman et al., 1997). Numerical ice sheet models, which attempt to quantify ice dynamics in order to reconstruct paleo-ice sheets or forecast future glaciations, can be divided into deduction models (Huybrechts, 1986; Boulton and Payne, 1992; Fastook and Holmlund, 1994; Takeda et al., 2002; Tarasov and Peltier, 2003, 2004) and inversion models (Tushingham and Peltier, 1992; Peltier, 1993; Lambeck et al., 1998). These methods have been augmented by improved computing capabilities, and also by the capability to reconstruct basal thermal conditions (Huybrechts and T’siobbel, 1997; Pattyn, 2003) and couple models to a variety of localized or global data (e.g., sea level, GRIP curves). Geologic and geomorphic methods utilize both marine and terrestrial landforms to reconstruct the timing and extent of paleo-ice sheets. For example, isostatic rebound (Lambeck, 1993; Kaufmann et al., 2000) and the use of glacial lineaments (drumlins, striae) and end moraines can be used to reconstruct the spatial extent of ice sheets (Boulton et al., 1985; Dyke and Prest, 1987; Kleman et al., 1997; Clark et al., 2000); various sediment data, including varve deposits (Litt et al., 2001; Breckenridge et al., 2004) and ice rafted debris (Broecker, 1994; Hindmarsh and Jenkins, 2001), combined with radiocarbon applications to date sediment sequences (Olsen et al., 2001) and cosmogenic radionuclide dating techniques to constrain erosional landforms and glacial moraines (Fabel and Harbor, 1999), also assist the reconstruction of the timing of ice sheet growth and decay. Separately, these methods offer unique, but limited, glimpses into the extent and behavior of previous glaciations and, despite numerous methodological and technological improvements within these methods, the models are rarely integrated in any systematic or quantitative manner for calibration or verification purposes. Integrating these methods has great potential to improve contemporary knowledge of previous and future glaciations, as well as our understanding of ice sheet dynamics.

The challenge with comparing geomorphic data against numerical models is designing a technique for the systematic comparison and statistical assessment of the level of correspondence between various models (e.g., numerical, geomorphic, geologic) of spatial and temporal patterns of ice sheet history. Thus, the motivation to develop this technique arose from the necessity to verify numerical ice sheet models using various field observations. There is a continuing demand to merge empirical data (e.g., end moraines indicating ice extent and lineations indicating flow direction) into modeling efforts (Clark, 1997; Kleman et al., 1997; Clark et al., 2004; Ehlers and Gibbard, 2003; Kleman et al., 2004; Napieralski, 2005), but previous efforts typically compared model output to field observations in a qualitative manner (Hubbard et al., 1998; Hubbard, 1999; Näslund et al., 2003). Modelers are certainly concerned with the level of agreement between their output and field observations (Andersen, 1981; Boulton et al., 1985; Boulton and Hulton, 1995; Boulton et al., 2001; Dyke and Prest, 1987; Hughes, 1998; Arnold and Sharp, 2002); they now have the opportunity to apply spatial statistics and Geographic Information System (GIS) capabilities in a sophisticated manner to quantify the level of agreement (Napieralski, 2005).

Many glacial landforms have unique spatial relationships that can be used to reconstruct paleo-ice flow patterns, potential basal thermal conditions, and the behavior of ice streams, and these relationships have been assessed using GIS (see Napieralski, 2005). For example, some of the first GIS were used to construct rose diagrams to illustrate primary and secondary flow patterns derived from field observations (Punkari, 1995). This system was recognized as a productive means for locally comparing numerically modeled output against conceptualized geomorphic models while reconstructing ice flow directions from the Fennoscandian ice sheet (Näslund et al., 2003). Recent GIS applications have focused on statistically analyzing the physical characteristics (e.g., spacing, length, conformity) of glacial lineations (e.g., drumlins) to delineate ice flow patterns and ice streams (Clark and Wilson, 1994; Clark et al.,
In addition, numerical ice sheet models have also been calibrated with empirical data by using various known ice-free interstadial localities to “force” the model to be ice free during the corresponding intervals (Näslund et al., 2003; Tarasov and Peltier, 2003, 2004). Although the geographical extent of modeled output has been compared to the geologic record, most of the results were simply reported as “underestimated” or “overestimated” (e.g., Siegert et al., 2001).

Verifying numerically derived model output with field observations can include various aspects that help constrain the extent, basal and ice flow patterns, and the timing of ice sheet growth and decay. This paper provides a methodology to evaluate the level of correspondence between modeled ice extent and the distribution of end moraines, generally regarded as a high priority in the comprehensive verification of modeled outputs using field evidence. Few previous efforts have attempted to describe the level of correspondence between various model outputs, with the overall objective of finding an optimum model that best agrees with empirical data. Therefore, the goal of this paper is to present Automated Proximity and Conformity Analysis (APCA), a new, GIS-based technique that compares the extent, and geometry, of model outputs by producing a proximity and conformity diagram (PCD). Through an iterative process, modeled output is compared against various field observations to ascertain which output agrees best with empirical data and, as a result, which input parameters produce the most accurate model. An overview of the method and issues will be followed by two examples to demonstrate various interpretations and approaches.

2. Methodology

The level of correspondence between linear features can be established by using a system of buffering and overlay and is conveyed in two general ways: proximity and parallel conformity. Buffering involves the generation of a new object which is within a specified distance of a point, line, or polygon, while an overlay is the combination of two or more map components to produce a new, additional layer (O’Sullivan and Unwin, 2003). Here, proximity is defined by the spacing between linear (but not necessarily straight) features, while parallel conformity is the angle between the same linear features (e.g., parallel, at some angle, or perpendicular). Multiple buffers are generated around the modeled output and one buffer around the empirical data, which are then merged into one feature (Fig. 1). Since the buffer rings increase in value from the model feature outward, the associated multi-ringed buffer values indicate the proximity of one feature to the other. A proximity value, which indicates the nearness of each buffer ring to the field observations, is calculated for each multiple buffer ring. If the end moraine is adjacent (and parallel to the modeled ice extent, the analysis will produce low proximity values. As the modeled ice extent departs in proximity from the end moraine, the proximity values will likewise increase. The cumulative plot of proximity values is used to illustrate proximity variation in the form of a PCD (Fig. 2).

The parallel conformity between two linear features is reflected by the slope in the PCD. All other factors being equal, a steep slope indicates relatively close parallel conformity between the features (Fig. 3). If the features are perpendicular to each other, then each multiple buffer ring will contain the same amount of buffer area from the field observations and, as a result, the slope of the PCD nears 45° (Fig. 4). This method can be implemented in many GIS environments. Here we use ESRI’s ArcGIS® and Arc/INFO® to illustrate the basic steps of this verification method (Fig. 5).
2.1. Data preparation

The data (model and empirical) needs to be in a common format and then merged into a geodatabase. The first step is to convert the data into a common format and then merge into a database. For this study, the model output and field data were converted to vector format. While most field data may already be in vector format, model output typically have to be converted. Once the data are in identical formats, and the features of interest are extracted (e.g. modeled ice extent with corresponding end moraines), the next steps of the comparative analysis can be performed.

2.2. Buffering

ArcGIS's buffering tool generates buffers of a fixed distance, extending both inwards and outwards from the features. The tool generates buffers of a fixed distance, extending both inwards and outwards from the features.

Fig. 2. Proximity between linear features is reflected in proximity and conformity diagram (PCD), which relates cumulative buffer area to buffer distance.

Fig. 3. Slope of PCD curves are graphed against angle between linear features and results show that steepness of PCD curve is directly related to angle between linear features.

Fig. 4. Angle between linear features is also illustrated in proximity diagram. As angle between linear features increases, slope of line decreases until it nears 45°.

Fig. 5. Overall procedure of comparative analysis using ArcGIS and Arc/INFO, illustrating data preparation, statistical operations, and output.
features of interest. Multiple buffers are generated around the modeled ice margin position (to provide an indicator of distance from modeled ice extent and the end moraine) and one buffer is generated around the end moraine (Fig. 6b). The buffer width has a considerable impact on the analysis and should be chosen with care. Buffer width should be based either on a specific distance that is utilized throughout the analysis, or a ratio of the feature being buffered (e.g. buffer width always equals 1/10,000 the diameter of the ice sheet) when that feature varies in size during the analysis (e.g. verifying deglaciation stages of continental ice sheets). For the examples in this paper, a specific unit of distance is used and, in this case, the width of the individual buffers is based on the need for sensitivity. The smaller the buffer width, the more likely that subtle change in proximity and conformity can be observed (a small buffer ring width reflects more subtleties than a larger buffer width, however increases computing time and data space). The multiple buffers should completely overlap the other buffer; thus, the maximum distance between modeled output and end moraines is the key factor when determining number of buffers. Only one buffer is generated around the field observation and the buffer width will impact the ability to observe subtle changes (a large buffer has more area to allocate than a small buffer).

2.3. Overlay (union)

ArcGIS geoprocessing capabilities were used to combine features from the two buffer layers into one feature, while still maintaining the original features and attributes (Fig. 6c). This was accomplished using ArcGISs Union tool and the resulting attribute table relates area to either one of the original buffers or where the two original buffers overlapped and were unionized. The unionized area is then extracted and analyzed in the PCD, which is used to determine the level of correspondence between features.

2.4. Data analysis

Area-percents of the field observation buffering polygon intersected with different buffer rings of modeled margins were calculated through an AML program (downloadable at http://www.iamg.org/CGEditor/index.htm). The accumulated area-percents and corresponding buffer distance are plotted in a proximity diagram, which illustrates the results from the proximity and parallel analysis.

3. Application of technique

To illustrate the application of this approach, two examples are used. The first example will compare various model outputs against a single, continuous end moraine to determine which output best agrees with field observations. The second example will demonstrate the various approaches to determining the best fit between various modeled output and multiple field observations (e.g., several end moraines).

3.1. Evaluation of different ice sheet models

Three modeled ice extents will be compared against the same end moraine in order to determine which model output agrees best with the empirical data (Fig. 7).

A multiple buffer, composed of 30, one-kilometer wide rings, are generated around three different modeled ice margins and a buffer of 5 km width was generated around the end moraine. Thirty buffers were chosen to ensure that the multiple buffers completely overlap the end moraine buffer. Each set of buffers were converted to ESRI coverages to maintain the specific attributes of
the features, and then unionized (consisting of one model output and the end moraine). The aim was to determine the “best fit” between modeled ice margins and an end moraine and three results can be ascertained: (1) model C is best overall fit, (2) model B has poor proximity but good parallel conformity (steep slope), and (3) model A alternates between good and poor parallel conformity (alterations in slope reflect changes in angle between features).

The PCD reveals the level of parallel conformity between model output and the end moraine. The modeled ice extent for model A (Fig. 7) has the same general shape as the end moraine, but is shifted to the right. This observation is also reflected in the graph, as the slope can be divided into unique segments: the initial steep slope (reflecting the near parallel conformity along the right half of the moraine), then a gentle slope (reflecting near-perpendicular proximity along the middle of the moraine), followed by a relatively steep slope (indicating the relatively good conformity, but poor proximity, along the left side of the moraine). The steep slope for modeled extent B (Fig. 7) indicates good parallel conformity (though poor proximity), while the slope for model C reflects close proximity and relatively good conformity. Thus it is possible to use the PCD to distinguish which models best agree with field observations in terms of proximity and parallel conformity.

Two approaches can be used to quantify the level of correspondence between linear features. First, the area under the PCD curve reflects the overall level of correspondence between model output and field data. Therefore, a single value can be used to indicate the combined effects of proximity and conformity, such that larger areas under the curve occur when there is both good proximity and conformity, there is a large area under the curve. This approach is the most useful and efficient means for quantifying the level of agreement between linear features because a single value describes the overall level of correspondence.

Second, distance and percentage thresholds can be used to differentiate between multiple model output that exhibits varying proximity and conformity, respectively. The buffer distance at a specified threshold, such as 70% or 90%, can be used to quantify the level of conformity. For example, the graph for model C crosses 70% at a lower buffer distance than the other models, indicating that, in regard to conformity, model C obtains more area within a specific percentage (steeper slope). The best fit can also be determined by specifying a buffer distance (perhaps derived from the modeling resolution or a previously determined, acceptable level of “error”) and ascertaining the percentage of buffer area within that distance. If, for this example, a 10 km buffer distance is used, then modeled ice extent A has 60% of the end...
moraine buffer within 10 km of the modeled output, model B has only 3%, and model C has 75% (Fig. 7). According to this approach, model C has obtained a better proximity than the other output. Though the distance chosen may also be somewhat arbitrary, to prevent conflicts, several buffer distances must be utilized in the analysis. The threshold employed must be chosen cautiously, as the impact on the analysis is not inconsequential. For example, thresholds of 70% and 90% can yield two different results (see model A and B in Fig. 7). Part of this problem derives from one model having good parallel conformity but poor proximity (model B in Fig. 7), and the other having good conformity but poor proximity (model A in Fig. 7). In this situation, the slopes of both graphs intersect and using one threshold to determine “best fit” produces multiple interpretations. In order to resolve this conflict, multiple thresholds, such as 50%, 70%, and 90%, must be utilized. For the same example, the buffer distances at these percentiles are 8, 20, and 28 and 21, 23, 27 for model A and model B, respectively. Of these two, neither has both good proximity and good conformity, but model A possesses the best overall level of agreement. Using the area under the curve, however, would clearly show Model A corresponds better than Model B.

3.2. Evaluation of model output using multiple field observations

When verifying multiple model outputs against multiple end moraines, there are two techniques that can be implemented to determine the optimum model. First, a comparative analysis is conducted as described in the previous example but the result is a cumulative “goodness of fit” (sum of proximity values and parallel conformity) for all end moraines. When comparing two modeled ice extents against multiple end moraines, it becomes difficult to visually determine which model output agrees best with field observations (Fig. 8). Thus the analysis is performed as described in the preceding section, but the proximity value reflects the overall level of agreement between each model output and all the end moraines (see graph in Fig. 8). This method can be used to rank various model outputs according to their correspondence with field observations, as well as quickly analyze large numbers of model outputs.

However, in many circumstances, a modeler may be concerned with the level of correspondence within specific geographic areas of the model output (e.g., level of agreement in broad, gently sloping regions vs. mountainous areas). In this case, rather than analyzing the overall level of agreement, each end moraine is buffered and analyzed separately to determine the localized level of agreement. The results indicate which segments of the ice sheet agree with (e.g., model B has a better correspondence than model A with 7 of the moraines) or deviate from (e.g., moraines 6–10 for model A) empirical data because the proximity values for each end moraine or groups of end moraines are analyzed and reported individually (Table 1). An understanding of the level of correspondence between modeled ice extent and end moraines within specific subdivisions of the ice sheet may indicate what model parameters need to be adjusted.

4. Discussion

Essential attributes of this method include relative simplicity and flexibility. Since verifying an ice sheet model may be an iterative process, it was critical that a
straightforward and efficient method be implemented. This became an issue when dealing with substantial amounts of spatial and temporal datasets, such as those associated with ice sheet modeling efforts. Output for this analysis, typically in vector format (though raster can be used), is relatively easy to maintain and store. The APCA approach is also accessible to GIS-users, since most GIS software packages offer the geoprocessing tools required for this process.

APCA is flexible in design and application, as the analysis can be customized to fit specific needs. For example, output from ice sheet models tend to cover vast spatial areas and the offset between model output and field data will typically be measured in kilometers or miles (thus the buffer widths). However, using APCA to compare landslide modeling output against landslide scars will most likely require the offset to be measured in meters, or less. Whether working with macro-scale or micro-scale modeling efforts, APCA can be customized to address these spatial differences.

Furthermore, if the same buffer characteristics (width and number) are utilized, APCA scores from multiple studies can be compared, and is not limited to numerical models. The buffer widths should be chosen upon modeling resolution, level of uncertainty (error in data), and data management issues. If the model resolution is 10 m, selecting a buffer width less than 10 will provide no more reliable insight than if using 10 m. Thus, resolution becomes a limiting factor when selecting buffer widths. However, the affect of various buffer widths on the PCD is minimal, as the PCD curve for the smaller buffer is more irregular, showing slight undulations that reflect changes in proximity that larger buffer will not identify. It is important to note that this has a minimal effect on the area under the curve, but may affect results from using thresholds. Finally, APCA also allows for any linear and polygonal features, such as lineations or frozen bed zones, to be analyzed as part of an iterative verification of numerical ice sheet models. As a result, areas under an ice sheet that may be preserved under frozen conditions (relict) throughout a glacial stage may be modeled and this technique can determine how well the modeled results fit the field evidence.

In the example that compared multiple model output against multiple field observations (Fig. 8), three thresholds were used to report the overall level of agreement and per individual end moraine. While this may seem arbitrary, a statistical analysis can be used to determine if a model, at any threshold, is (statistically) better than another model. The distribution of buffer distances generated at specific percentiles for multiple end moraines can be compared against the distribution of buffer distances drawn from other models to determine if the distributions are similar or statistically different. If statistically different, then one model can be considered better, at least in terms of proximity. While this process is typically accomplished using buffer distance (proximity), the angle between features (or, if the features meander, between feature trend lines) can also be used in

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<th>Moraine</th>
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<th>Model B</th>
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<tr>
<td>1</td>
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<td>St. Dev.</td>
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End moraines are labeled 1–10, counterclockwise from left to right around ice sheet. Distribution of buffer values can be used to determine if one model agrees better, or if a particular threshold produces a different result than another. Furthermore, the area under curve was calculated and is presented to show which model best agrees with each moraine. In this example, Model B corresponds better with end moraines than model A.

*Area under curve is also used to determine which model best fits each moraine.
order to determine which model produces the best conforms to field observations. In addition, the same tests can be applied to various thresholds to determine if there is a difference between those that are chosen. Naturally, in situations where there are only a few field observations, the capability to statistically analyze the distribution of buffer distances and angles is reduced.

The analysis also weighted the APCA scores for each moraine equally (Fig. 8). While this provides a good overall working example of APCA, there are several reasons to consider weighting APCA scores differentially when determining the overall level of correspondence of model output. As each moraine varied in size, this could be considered during the analysis by weighting the APCA scores according to moraine length. Models that correspond better with longer moraines might be weighted heavier than smaller moraines. Thus, for the example provided (Fig. 8), end moraine #6, clearly the longest, would be weighted more than #9, which is the shortest moraine. In other circumstances, it may be advantageous to weight moraines according to areas of interest in order to emphasize the need to match specific segments of the ice sheet with field data. For example, if an area of interest is located along the southern margin of an ice sheet, the southern moraines can likewise be weighted more. However, caution should be taken when using this approach as over-emphasizing margin matching in one segment of an ice sheet does not mean a realistic simulation has been produced since other portions of the ice sheet must also have some correspondence to achieve a realistic configuration.

Another important issue to consider is the chronologic uncertainty associated with dating techniques used to constrain end moraines. End moraines that have ages with greater uncertainty can be weighted less than those with a reduced amount of uncertainty. Consideration of this issue provides more realistic temporal constraints when comparing time slices of modeled ice extent against end moraines. If dealing with one moraine, it is important to determine when the “best fit” occurs. For example, an end moraine with an estimate deposition time of 15ky (+1000 years) can be compared against 16, 15, and 14ky to determine best fit. Whichever time slice agrees with the evidence best, must also agree with the neighboring end moraines, so as to keep retreat rates feasible. Thus, the verification of a time slice may be iterative, dependant on the level of correspondence with neighboring end moraines. If there are multiple moraines, the analysis can be weighted so that those with a greater uncertainty have the smallest bearing on the overall interpretation of the analysis. For example, if moraines (such as in Fig. 7a) have the same estimated year, but because dating techniques have different uncertainties, each would carry different weights so that the end moraine with the greatest certainty provides the most influence on the interpretation.

Furthermore, other field data, or even an ensemble of data, can be used to indicate the overall subglacial regime and the location and patterns of these features can be combined in an APCA. Landforms, such as relict zones (frozen bed patches) and eskers, can be linked together in an APCA to provide more spatial and temporal constraints in the analysis. Thus, the manner in which APCA is conducted is flexible, as the user can design the analysis to emphasize landforms or regions of the ice sheet that need to be accentuated or field data with less uncertainty.

5. Conclusion

The application of APCA provides glaciologists with a tool to evaluate the level of agreement between model predictions of ice margins and field data. Determining the level of correspondence between estimated ice marginal positions and end moraines may be only a portion of the overall verification process, but it is one that has limited modelers in the past because of the difficulties of measuring or quantifying the level of agreement between linear features. Once the modeled extent is in reasonable agreement with end moraines, then the ice flow characteristics and subglacial regime can be subsequently verified. Through this iterative process, an (or several) optimum model output is generated from a unique combination of numerical theory and field evidence. Results from the verified model provide data to assist the reconstruction of various elements of paleo-climates.

Although APCA is illustrated here in the context of verifying numerical model output against empirical data for ice sheets, the technique can be applied to a wide range of geoscience situations where it is desirable to determine how well model predictions of the spatial extent of some phenomena fit empirical data. For example, models that reconstruct debris flows, tsunami run-outs, and flood extent, may need to be verified against field observations that indicate the extent of these natural phenomena. APCA could be used to determine the goodness of fit between model and empirical data and, as a result, improve knowledge regarding the origin and dynamics of these features.

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