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Quantifying the role of individual sources of error and uncertainty in model validation: A case study in conductive heat transfer

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The process of model validation requires a priori assessment of both error and uncertainty in model implementation (theory and numerical implementation) and constitutive and closure relations. Here we stress that validation studies in solid earth simulations have rarely included formal uncertainty analyses of transport and thermo-physical properties. Given that Earth materials are usually multicomponent, multiphase ensembles with wide ranges in uncertainty, it is difficult to assess what constitutes robust validation. In this presentation we will expand on the formal definitions of error and uncertainty for application to heat and mass transfer models as exemplified in the context of canonical heat transfer by conduction.

We define error as a deficiency not due to a lack of knowledge, typically arising for reasons of practicality and tractability. They can be acknowledged errors, such as round-off, discretization, or convergence errors, or unacknowledged, such as programming errors. Uncertainty represents a lack of knowledge, and may be classified as either aleatory or epistemic. An aleatory uncertainty is due to the natural variability in known quantities, that cannot be eliminated or entirely accounted for, and are often treated with a pdf approach. Aleatory uncertainty is not due to a lack of knowledge, but from the fundamental inability to constrain a parameter outside a window of variability. Epistemic refers to a reducible uncertainty that is due to a lack of knowledge about the system, and may be improved by additional observations or measurements. Both types of uncertainty commonly occur in solid earth applications.

Both error and uncertainty contribute to issues with validation and prediction, complicating the assessment of verisimilitude. In solid earth simulation, little attention has been paid to the interplay between sources and magnitude of error and uncertainty. In our presentation we will demonstrate how global solution uncertainty can be decomposed, or at least quantified, by identifying the greatest individual sources of inaccuracy. We exemplify this approach by considering conjugate conduction where three physical properties, density, conductivity and specific heat capacity contribute to heat transfer. We will revisit and assess the validity of the claims of Whittington et al. (2009) who measured precise thermal diffusivity for five rocks from 300 K to 1250 K, applying the average of these values to global continental crust.