Strategies for Modeling Multi-Scale Systems

A. Brad Murray
Division of Earth and Ocean Sciences, Nicholas School of the Environment and Earth Sciences;
Center for Nonlinear and Complex Systems, Duke University

Introduction

To address how landscape-forming processes operate, and how they interact with human manipulations, we must grapple with multi-scale systems—systems in which diverse processes interact across disparate time and space scales. For example, in the nearshore environment, wave- and sand-grain motions with time scales of seconds form decimeter-scale ripples on the bed. These roughness elements affect the larger-scale currents and sediment transport that reshape nearshore bars and the beach over hours and days. These complicated interactions, operating during storms and fair weather, somehow add up to net alongshore sediment flux patterns that sculpt sandy coastlines. To investigate large-scale coastline changes and their two-way coupling with efforts to protect coastal development using a numerical (or analytical) model, what scale of processes should we explicitly represent?

Two end-member strategies for dealing with such modeling quandaries can be identified. In what I call the 'explicit numerical reductionism' approach (*Murray*, 2003), a modeler strives to represent processes on scales as small as is practical, parameterizing 'sub-grid scale' processes only when unavoidable. In contrast, using the 'top-down,' 'synthesist,' (*Paola*, 2000), or 'hierarchical' (*Werner*, 2003) strategy, a modeler treats interactions between variables defined at scales commensurate with those of the phenomena of interest; only the *effects* that processes on much smaller time and space scales have on the scale of interest are explicitly included.

Theoretical Contexts

The top-down approach reflects perspectives developed in complex-systems research. Often in natural (*Schweber*, 1993) and engineered systems (*Ottino*, 2004), relatively large-scale variables, interactions, and phenomena emerge from the collective behavior of many smaller-scale degrees of freedom, the way pressure, density, water-surface elevation, and surfing waves emerge from the not-quite-random motions of water molecules. The 'emergent phenomena' perspective suggests that the most appropriate way to understand and predict such systems is to address the interactions between the emergent variables, and that the study of the much smaller scale processes that give rise to the emergent variables should be considered to be a separate, although related, endeavor.

Chaos theory produced the enduring lesson that even very complicated behaviors can result from simple interactions. Therefore, to help explain and predict the behaviors of a messy, spatially extended natural and/or human system, a numerical model may not need to include a multitude of complicated processes at various scales, contrary to what intuition may suggest; a model treating only relatively simple, large-scale interactions may be more effective. A recent top-down coastline-change model provides an example, illuminating how complicated large-scale plan-view coastline shapes can emerge from simple, local interactions (*Ashton et al.*, 2001).

Rules vs. Established Parameterizations

When fluid flow, soil, and/or sediment are involved in a multi-scale system, models generally can't be built solely from basic physical laws; some level of parameterization is required. The effects of turbulence on sub-grid scales must be parametrically represented, and other parameterizations take the form of constitutive relations describing the rheology of a material, or relationships predicting bulk (many grains) sediment fluxes. Such parameterizations synthesize the effects that smaller-scale processes have on larger-scale behaviors. Parameterizations of this sort are often based on relatively small-scale laboratory experiments.

A researcher trying to construct a top-down model of a landscape-scale system often faces a lack of well-established parameterizations at the scale deemed most appropriate. The researcher may choose to devise a new large-scale parameterization based on observations, theory, or experience. Such hypothesized relationships are often termed 'rules.' This terminology, while differentiating newly proposed parameterizations from the well-tested ones, obscures the continuous nature of the spectrum between 'rule-based' and more traditional models. Rules, which can represent first guesses at the form of relatively large-scale interactions, are often not as quantitatively accurate as parameterizations based on a history of empirical testing.

Simplified Parameterizations and Explanation

When the goal of a modeling endeavor is to try to explain an enigmatic phenomenon, the approximate nature of a newly minted rule does not necessarily pose a problem. Along with leaving out many of the processes operating in a system, representing the interactions hypothesized to be important in a simplified form can increase the clarity of the potential insights the model can facilitate. Such highly simplified 'exploratory' models (*Murray*, 2003) provide a useful first step in untangling the key mechanisms in a complex system. They must be followed up with appropriate tests of whether the interactions in the model are the ones that are important in the natural or human system (*Murray*, 2003). Nonetheless, the basic understanding that exploratory models foster is a prerequisite for informed engineering and management decisions.

Model Scales and Prediction

Even though predictions of specific future occurrences is generally not possible, engineers, managers and planners prefer models that produce more precise, numerically accurate predictions of typical system behaviors than exploratory models are designed for. Is the top-down strategy useful in this context? Or will explicit numerical reductionism produce more numerically reliable predictions?

The answer depends partly on the complexity of the system; systems involving a limited range of scale are likely to be more amenable to explicit numerical reductionism. However, when interactions between processes spanning a wide range of scales are important, a bias toward basing a model on the very small scales can lead to inaccurate predictions; inevitable imperfections in the small-scale-process model components can add up to unrealistic behavior at larger scales (*Werner*, 2003; *Murray et al.*, 2005). Basing a model on the interactions that emerge on scales not much smaller than those of interest avoids this potential pitfall.

Alternative approaches to modeling inner continental shelf sea-bed patterns exemplify these points. Striking kilometer-scale grain-size sorting patterns have come to light all around the world as side-scan sonar technology has become widespread (*Murray and Thieler*, 2004). Murray and Thieler (2004) hypothesized that a simple feedback, and subsequent emergent interactions produce the arrangements of sharp-edged domains of alternating coarse and fine sediment. The hypothesized feedback involves how wave-generated ripples affect larger-scale sediment transport where waves and currents interact. Murray and Thieler constructed an exploratory model to test the plausibility of the hypothesis, representing the key interaction with a rule that represents the effects on relatively large-scale (several meters) sediment fluxes produced by: 1) ripples forming with dimensions that depend on wave and grain-size characteristics; 2) how these ripples interact with wave motions to produce a vertical suspended-sediment profile; and 3) how mean currents advect that suspended sediment. The simple rule related large-scale sediment flux directly to bed composition, as a proxy for the well-documented formation of larger ripples where the bed was coarser, and the resulting cascade of effects. The exploratory model did produce sea-bed patterns with characteristics matching those in nature, and the simplified interactions in the model enabled analysis of the model behaviors (*Murray and Thieler*, 2004).

In a subsequent attempt to reproduce the results in a more numerically accurate model, a model was developed that treated the small-scale details of ripple formation and vertical profiles of suspended sediment and currents (*Murray et al.*, 2005). Experiments with this model showed that the available parameterizations at smaller scales, derived largely from laboratory-scale experiments, were not accurate enough in the field context to produce reliable results; combining different empirical or semi-empirical predictors of the smaller-scale quantities produced very different results. With some combinations, the key observational fact that larger ripples and sediment fluxes occur where the bed is coarser did not emerge. To produce a numerically accurate model, two options are possible: Many researchers can work for a long time to improve the small-scale parameterizations. Or, through appropriate field experiments, an empirically grounded larger-scale parameterization can be developed—one that represents the lumped effects of the smaller-scale interactions. The latter approach will insure that the relatively large-scale interactions in the model faithfully represent those in nature.

The top-down and explicit-numerical-reductionism modeling strategies are merely end members, and most of the models we all construct fall somewhere in between. When trying to model a highly complex system, we should keep our minds open to devoting more of our efforts to developing larger-scale parameterizations that synthesize the effects of smaller-scale interactions—such efforts could lead more efficiently to increasingly accurate predictions of system behaviors.

REFERENCES

Ashton, A., Murray, A.B., and Arnoult, O., 2001, Formation of coastline features by large-scale instabilities induced by high-angle waves, *Nature,* **414,** 296-300.

Murray, A.B., 2003, Contrasting the Goals, Strategies, and Predictions Associated With Simplified Numerical Models and Detailed Simulations, *In* (Eds, Iverson, R.M. and Wilcock, P.R.) *Prediction in Geomorphology*, Vol. 135: AGU Geophys. Monogr., pp. 151-165.

Murray, A.B., Coco, G., Green, M., Hume, T.M., and Thieler, E.R., 2005. Different approaches to modeling inner shelf sorted bedforms, *4th International Symposium on River, Coastal and Estuarine Morphodynamics,* Champaign-Urbana, in press.

Murray, A.B., and Thieler, E.R., 2004, A new hypothesis for the formation of large-scale inner-shlef sediment sorting and 'Rippled Scour Depressions', *Continental Shelf Research,* **24,** 295-315.

Ottino, J.M., 2004, Engineering complex systems, *Nature* **427,** 399.

Paola, C., 2000, Quantitative models of sedimentary basin filling, **47**(Suppl. 1)**,** 121-178.

Schweber, S., 1993, Physics community and the crisis in physical theory, *Physics Today,* **46,** 34-39.

Werner, B.T., 2003, Modeling landforms as self-organized, hierarchical dynamic systems, *In* (Eds, Iverson, R.M. and Wilcock, P.) *Prediction in Geomorphology*, Vol. 135: AGU Geophys. Monogr., pp. 131-150.