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Notes on "Modeling, Simulation and Analysis of Complex Networked Systems"

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Abstract

This is meant as a place to put commentary on the whitepaper[2] and is meant to be pretty much ad-hoc. Because the whitepaper describes a potential program in DOE ASCR and because it concerns many researchers in the f eld, these notes are meant to be extendable[1] by anyone willing to put in the effort. Of course criticisms of the contents of the notes themselves are also welcome.

[1]The TEX source[**?**] is available for this purpose, please start your own section under your own name to keep things a little organized.

1 Rob Armstrong's Notes

1.1 Introduction

This is a well thought out program plan and a good direction for SC research in complex systems. This is said in preface to comments that might be construed as criticism but is rather an attempt to clarify and give depth to terms and concepts introduced in the white-paper. The directions that the white-paper puts forward are appropriate and answer a long-term need.

1.1.1 History

While this area is relatively new as a subject in mathematical physics. Modeling and simulation of complex systems in operations and systems research, including the energy economy has been around for a long time [1]. Efforts in the commercial and research arenas arguably dwarfs that of traditional scientif c computing. Discrete Event Simulation (DES) and Agent-Based (AB) modeling are usually the tools of choice for modeling practical complex systems (as they are usually employed, the former could be considered a special case of the latter). Yet the mathematical underpinnings that might relate entity models and interconnection topologies are largely missing. Often experimental results are impractical or too expensive for the physical systems of most interest. Lacking any guidance from mathematical physics, behavior can only be exampled at full scale. For example, understanding the impact on stability of a even a seemingly minor change in the electrical grid is not practical nor desirable experimentally. Lacking the def nitive experimental evidence of overall behavior and the mathematical underpinnings to extrapolate to scale, designers of such simulations often consider the "better" model to be one for which as much detail as possible is loaded into the entities and their connections. Because they lack these tools, this is done without a clear understanding of each parameter's dependence in the emergent behavior of the overall system nor its interdependence with other parameters.

1.2 Observations

The whitepaper makes a number of attempts to distinguish between the simulation of complex systems and the sort of simulation that is common in the science domain. Variously complex systems are characterized by "networks of discrete components" [2] (the statistical mechanics of an ideal gas is a counterexample that would not be considered complex) and distinguished from "physically based systems" [3](all of the example in the whitepaper are physical). Another adjective used to characterize complex systems is "surprising" and "emergent"[4]. (Even a simple, non-complex, example from quantum mechanics exhibits emergent behavior that surprised Einstein). Although

[2]Page 1, Line 2
[3]Page 1, Line 9
[4]e.g. Page 3, under the f rst bullet.

these features *are* often cited [5, 6] as a signs that the physical system is complex, they are rather unspecif c and a more precise distinction might be more satisfying.

In general, mathematical physics over the previous century has recognized two approaches to describing physical systems:

1. Systems that are well represented by a phenomenalogical equation of evolution. This includes PDE's. ODE's, etc. (e.g. quantum mechanics, transport phenomena).
2. Systems for which a statistical average determines the emergent behavior of interest. This applies to phenomena for which its constituent entities are loosely coupled or for which an ergodic principle exists. Here each entity contributes a proportionately to the overall behavior. This includes thermodynamic systems, but specif cally excludes any behavior that is self similar or scales with the size of the system, such as a 2^{nd} order phase transition.

But there also exists another category that has received little attention until recently:

3. Emergent behavior of a large system of entities that is not the result of a statistical average of individual contributions. Unlike systems reducable to classical statistical mechanics, the modif cation of a small subcollection of entities does *not necessarily* produce a proportionately small change in the emergent behavior. Contrarily, if every such small subgrouping does contribute a proportionately small effect, then it is reducable to item 2 above. If only a small subset of entities come to dominate the emergent behavior (albeit nonlinearly) then the system is reducible to item 1. Only if a scalably large subset of entities contributes in a strongly coupled fashion such that perturbations to small subset causes order zero changes in the result *and* no f nite (i.e. nonscalable) subset of entities is suff cient to describe the overall behavior, then the system should be regarded as "complex".

The overall behavior of complex systems is determined by strong nonlinear entity interactions like 1 above but also scales with system size like 2. Unlike 1 above the emergent behavior is the result of a large scale system (albeit, in principle reducable to PDE's or ODE's) and unlike 2 above the emergent behavior is not the result of an incremental contribution from weakly coupled entities. Rather than viewing entities as an ensemble of molecules as in a thermodynamics each contributing more or less individually, entities in a complex system are better viewed as lines in a computer program. Altering any line or group of lines can, and generally will have a dramatic effect on the output.

Indeed there is a strong association in the literature [6] with computational ability and complex systems. Particularly in the context of adaptivity in evolved [5] or "highly designed" systems [3]. This class incudes engineered systems that have arrived at an organized condition by human design much as highly evolved organisms might. Many investigators [4] feel that the Internet, national electric power grids, social systems and economic systems are examples of such complex systems. On the other hand there is some dissention from this viewpoint. At the center of the controversy is two different ways of viewing complex systems, both mathematically valid, but have widely differing consequences in their abstract interpretation and physical mechanisms.

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