Molecules for Modelers

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Purpose

Molecules are the building blocks from which good system dynamics models are built. By delineating and organizing molecules we are creating a new body of knowledge that will make it easier to learn modeling and provide a vehicle for focused discourse on the nature and quality of model formulations. By implementing these ideas in software we make it faster and easier for novice and experienced modelers to develop high quality system dynamics models.

Background

Developing the skills to create good system dynamics models takes many years. Few, unfortunately, have that much time to devote to study. Once a person has come to grips with the ideas of feedback, structure and behavior they are often called upon to use that knowledge by developing a simulation model. Lacking a breadth of experience the development of such models is difficult and slow with the resulting model often of less than sufficient quality.

Much of the difficulty in developing models stems from the requirement that the modeler abstract from a problem sufficiently to get a concise and usable formulation. As an example, consider the problem of determining the average skill level of workers in a factory. The correct, concrete, way to do this would be track each individual worker. Since this is not practical, a reasonable dynamic approximation might be an aging chain. An alternative, and more compact representation, would be a productivity coflow (a coflow with a learning effect). Knowing which of these to choose is a judgment that requires some skill to make. Knowing that these two options are available requires some exposure to the concepts in formal training, review of other models or reinvention of the structures.

Molecules and their organization provide a structured and reliable way of presenting important and commonly used elements of structure to learning and experienced model builders. By having access to tried and true formulations modelers can review what has been done before and modify or directly incorporate these formulations into their own models.

Stocks, Flows and ...

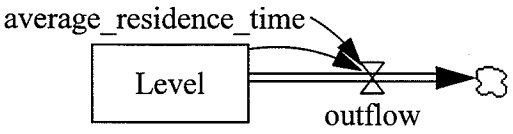
At a very early stage in learning model building, normally before a single equation is written, people learn the difference between stocks and flows. Finer distinctions, and other concepts such as auxiliaries, constants and lookup tables are also typically introduced. After this most teaching is done by example, with no usable taxonomy presented for going further. This is very much like providing a clear explanation on wood and nails and then letting students watch a house being built in order to learn how. While this might work, it would clearly be a slow and inefficient method for teaching people how to build houses.

Just as there are standard substructures and assembly techniques used in building houses, there are frequently recurring and nearly standard substructures used in building models. Some of these, such as first and third order delays (Forrester, 1961) and coflows (Hines 1983, Homer 1983) have been documented and explicitly discussed. Most, however, remain implicit, part of the knowledge base that each individual develops.

Molecules

We have chosen to call these elements of structure "molecules." Molecules are built up of the primitive stock and flow elements and are, in turn, the building blocks of complete models. The analogy with chemistry is not complete, but the name does convey much of the spirit of what is being captured.

One of the simplest molecules, and one that probably appears in most models, is the decay process.



$$Level = \int(-outflow)dt$$

$$outflow = \frac{Level}{average\_residence\_time}$$

For a simple molecule such as this it is probably easiest to simply check the form and enter the equations directly instead of trying to directly incorporate part of all or it. In general, however, it will be easier to cut and paste or inject molecules into a model and make the appropriate modifications to appearance and naming conventions.

Since components of molecules (for example the level in the above example) may already be in place, there needs to be flexibility on how much of the molecule to include. Thus, even though we think it is best to present molecules as complete dynamic models, we do not expect all of this to be used when building models with molecules.

Molecules and Objects

Molecules are closely related to what are called "Classes" in object oriented programming. The material delay is a molecule that is derived from the decay molecule and the material delay is used in the aging chain discussed in the background section. Similarly the productivity coflow is derived from the standard coflow which is derived from a smooth (Hines 1983). This object oriented organization is very helpful because it provides a very good way to learn about successively more complicated molecules. Once a molecule is thoroughly understood, it is a much easier task to understand the molecules that derive from it and use it.

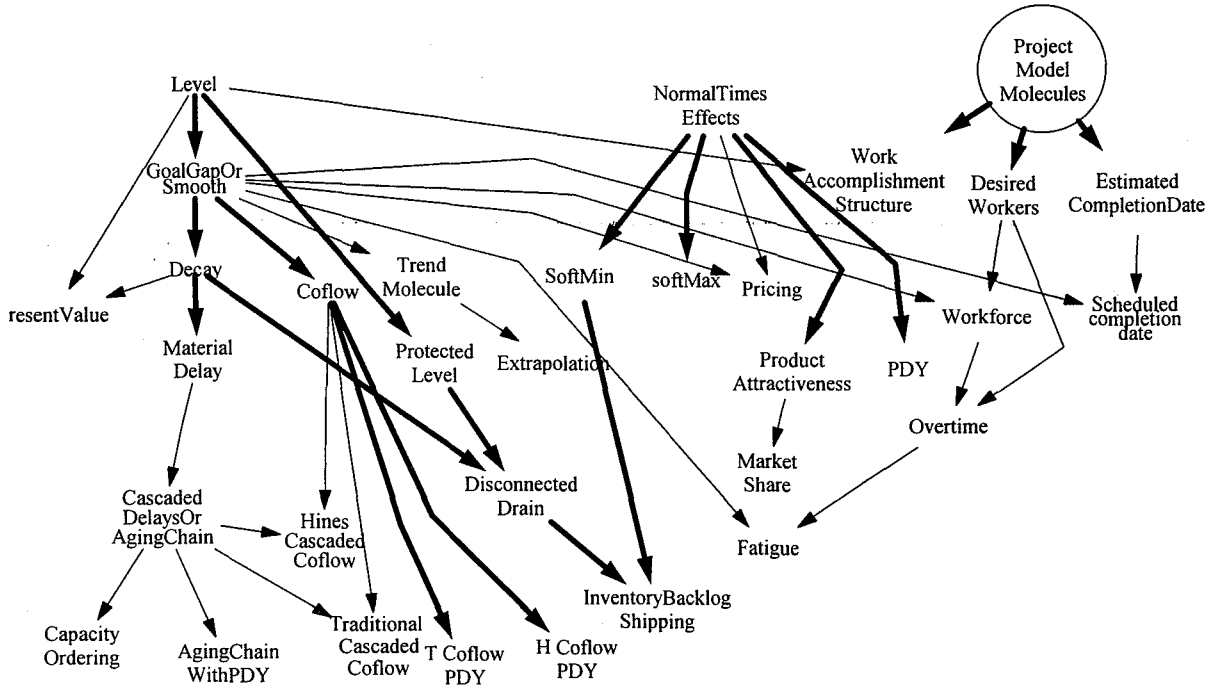
Molecules and Archetypes

It is useful to draw a distinction between molecules and archetypes (Senge 1990). Archetypes present dynamics lessons that have been learned from systems having certain structural characteristics. Molecules are building blocks from which structure is created. Their purpose is to improve the ability to represent structure, not draw lessons from particular structures.

A Taxonomy

The following diagram represents a preliminary selection of molecules and their relationships. We have used thick arrows to indicate that the molecule at the end of the arrow is a specialization of the molecule at the beginning of the arrow. The thin lines are used to indicate that the

molecule at the end of the arrow makes use of at least a portion of the molecule at the beginning of the arrow.



Software Implementation

Ultimately, we intend to implement the molecule framework as a stand-alone application that will allow users to look up, experiment with and classify molecules in a number of different ways. The molecules themselves will be usable with system dynamics software supporting the model interchange format (MIF) protocol (Myrtveit 1995). This will allow anyone doing system dynamics models to make use of the molecules.

The current implementation of molecules has been done as an add-on to Vensim®. The diagram displayed above is presented when the user selects a special menu item. Double clicking on any of the named molecules in the diagram brings up that molecule. The user can then select the portion of the molecule that they want, copy it into the clipboard, and insert it into the model they are working on. Once this is done the normal Vensim tools are used to rename the model elements and change the units of measurement.

Results

We have been using molecules informally in workshops for several years now. To our surprise, we have discovered that by simply giving them a name and claiming that they exist people become much more interested in them. Thus, as we have begun to present these ideas in a more structured format we have been rewarded by the appreciation given to the ideas. During the building of models people will repeatedly refer to the lists of molecules that have been presented to them even though, until recently, they have not had a good mechanism for finding a molecule relevant to a particular problem.

The taxonomy and current Vensim implementation presented in this paper have been used by one of the authors (Hines) for the second system dynamics course taught at MIT and has met with a great deal of enthusiasm. Students have been using the molecules as a means of making progress

in building models and have a very strong enthusiasm for the whole concept of molecules. In addition, the molecules have proven to be the easiest way to organize the presentation of more advanced topics and, at this point, seem like a necessity for the presentation of this information.

Continued Work

The development of molecules is a project that is continuing. We are currently faced with the recognition and classification of molecules that have been broadly used in the past. It is clear, however, that as modeling work continues new constructs are developed and some of these can usefully be recognized as molecules. As the classification becomes more refined there will be many opportunities for more specialized molecules and their organization will provide a very clean way to capture new formulations and to communicate them efficiently to other modelers.

Conclusions

System dynamics remains, for many, a dark art. The key to building good quality system dynamics models is the recognition and incorporation of important feedback loops. Since feedback is, by its very nature, non compartmentalized most of the standard mechanisms, such as sectors, for organizing models are of limited use. Molecules provide a new way of organizing both our models, and our knowledge about building models that give beginning modelers access to important guidance in the model development process, speed the modeling process for experienced modelers and improve the quality of discourse on formulation issues.

Beyond pedagogy, the steady extension and improvement of our models has been hampered by not being able to work on modeling as a series of small, solvable problems. Instead we focus on the whole model and solve formulation issues in this context. Molecules and their organization offer a better way. The debate about, improvement on, and creation of new formulations now can occur in an environment focused narrowly and cleanly on these important matters. Larger discussion sparked by the larger models also benefit, because that discussion can move cleanly away from the micro consideration of "molecular" formulations and onto the macro issues of dynamics.

Acknowledgments

The development and classification of molecules is an activity that many people, in addition to the authors, have contributed to. In the work so far significant contributions have been made by: Richard Ho, Dewey Johnson, James Melhuish and George Richardson,

Much of the inspiration for this work comes from the "cookbook" ideas on model building presented by Barry Richmond and Steve Peterson in the early Stella manuals.

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