Appendix A – Examples

A.1. What This Appendix is About

Equations 3.1 and 3.2 provide a mathematical framework for describing systemness and provide the guidance for functional/structural decomposition of systems of interest (Chapter 5) as well as to the construction of a knowledgebase for the system (Chapter 7).

In this appendix we will demonstrate the usage of these equations starting with a simple (one of the simplest) system, the deuterium atom, a hydrogen atom with a neutron in the nucleus. We show how the components and relations are captured, how the system interacts with its environment, and how the internal components can be further decomposed.

From the atom we move to a molecule, water in this example, to show how combinations of atoms form and provide emergent properties. This example is still fairly simple but begins to demonstrate the universality of systemness as the Universe evolved more complexity.

In both of these examples we provide discussions about more complex versions of each, i.e. heavier atoms and larger molecules, particularly proteins as enzymes and nucleic acids as stores of knowledge.

The last example is of a living cell, a prokaryotic cell (without a nucleus or membrane-enclosed organelle). With the advent of life, the level of complexity has become quite high. Yet, cells are made from molecules and atomic-level components. Here we see that complexity involves the way simpler molecules can interact to form macromolecular component subsystems and how these subsystems interact functionally to maintain the living system.

A.2. The Atom as System

A.2.1. Deuterium Atom

In this example we will use the subscript indicating the level of analysis, in this case level 1. In subsequent examples we will leave this notation off.

A.2.1.1. Components and Internal Network of relations (section 3.3.3.1):

C_1 = <P, 1}, {N, 1}, {e, 1}>; P = proton, N = neutron, e = electron; note the membership function is one, meaning always in the set.

N_1 = <C_1, L_1 >

L_1 = <{P, N}, {P, e}>

{P, N} is the residual strong force

{P, e} is the electrical charge force

A.2.1.2. Network of interactions with environmental entities (section 3.3.3.2):

$G_1 = \langle\{\mathrm{Src}_1, e\}, \{e, \mathrm{Snk}_1\}, p\rangle$

Where:

Src_1 is some distant light source

Snk_1 is effectively deep space anywhere

p is a photon. A photon of the right frequency interacts with the electron to change its state to a higher energy. When the electron emits another photon at a lower frequency the electron returns to its minimum energy state.

Other examples in G include higher quanta energies (e.g. that might ionize the atom) and direct physical interaction with other atoms resulting in a change in momentum.

A.2.1.3. Boundary (section 3.3.3.3):

$B_1 = \langle P_1, I_1\rangle$

P_1 = list of orbital shells (augmented with descriptions of geometries, energies, etc.)

I_1 = electrons in each shell

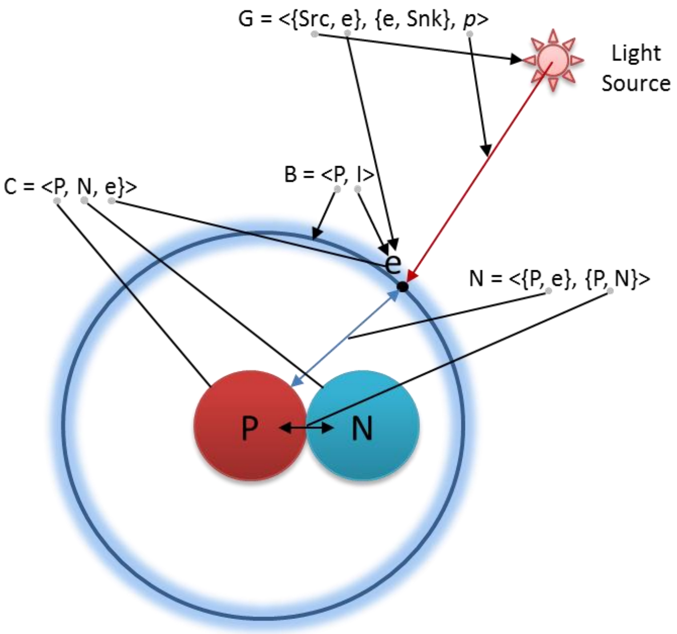

Fig. A.1. An atom is a system.

A.2.1.4. Transformation(s) with reference to the G interactions above (section 3.3.3.4):

$T_1 = \langle t_{1,1}, t_{1,2}\rangle$

$t_{1,1}$ = e + *p* -> e^ -> *p*v + e (^ is higher energy state, v is lower frequency – note energy is conserved)

$t_{1,2}$ = m_t -> m_{t+1} (m is a momentum vector, velocity and direction; the vector at time *t* and then at time *t*+1, using Δ*t* below.)

A.2.1.5 Memory or history (section 3.3.3.5):

The excitation state of electrons above the ground state provide a very short-term memory of the recent history of the atom’s interactions with its environment.

A.2.1.6. Δ*t* (section 3.3.3.6):

A time constant small enough to capture the dynamics of electron transitions? https://en.wikipedia.org/wiki/Atomic_electron_transition suggests nanosecond scale for the transitions so something like 100 picoseconds, though since the dynamics are essentially a step function, a picosecond or slightly more, depending on the shell, might be sufficient.)

A.2.1.7. Level 2 – Subsystems of Nucleons

Protons and neutrons, generically nucleons, along with electrons are subsystems of the atom. Following the systems analysis as per chapter 5 we would next decompose these components to produce a level 2 map/tree. Because we will find the fundamental particles to be (at least for now) non-decomposable (leaf nodes on the tree), level 2 is the terminal for the recursion.

The subsystems of protons and neutrons are quarks and gluons. As far as we know currently electrons cannot be decomposed (other than possibly to pure energy). Quarks communicate (are strongly bound) by the exchange of gluons (as flows of energy?) This ignores, for the moment, virtual particles that may be treated as a multiset of particles that have membership functions relating to coming into and out of existence.

The filling in of the C_2 and other structures is left as an exercise for the reader.

A.2.1.8. Onto/Combo-genesis

Thru nucleosynthesis in stellar fires and super novae explosions protons and neutrons are forced (in extreme temperatures and pressures) to combine.

A.2.2. Heavier Atoms

Components and Interactions are similar to the deuterium atom WRT: protons/neutrons/electrons. However, the proton set forms a center of charge with flow connections to all of the electrons. These flows are differentiated by virtue of the shells (energies) occupied so need to be enumerated thus.

For example, for helium-4 we have:

C = <{P_1, P_2}, {N_1, N_2}, {e_1, e_2}> ; subscript indexes indicate multiset identification not level.

and since the inner electron shell is full, and helium is “inert” the boundary conditions include an inability to share electrons as in covalent bonding.

A.3. Molecules

A.3.1. H_2O

We will look at another simple system, the H_2O molecule. This system is still ‘simple’ but more complex than the atoms of which it composed.

A.3.1.1. Components and Internal Network of relations (section 3.3.3.1):

C = <{H_1, 1}, {H_2, 1}, {O, 1}>; H = hydrogen, O = oxygen, C is a multiset with two hydrogens.

N = <C, L >

L = <{H, O}, {H, O}>; {H, O} is a covalent bond; hydrogen shares its single electron with one of the two spare ‘holes’ in oxygens second shell (which has space for 8 electrons).

Augmented by geometric considerations. E.g. the distance between hydrogen and oxygen nuclei is 95.84 picometers, the angle between hydrogens is 104.45 degrees. This latter is important since this causes the molecule to be polar, oxygen supplying an excess of electrons at the pole opposite the average hydrogen separation and the hydrogens providing a positive charge. See the G network.

A.3.1.2. Network of interactions with environmental entities (section 3.3.3.2):

Hydrogen bonds

G = <{Src, O}, {HH, Snk}, {e^-, p^+}>
Where:
Src is a positively charged atom or molecule
Snk is a negatively charged atom or molecule

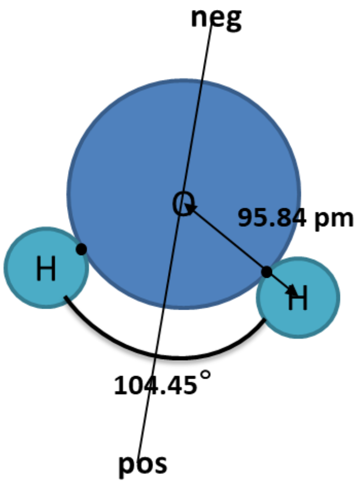

Fig. A.2. A molecule of H_2O shows new (emergent) properties of being able to interact with other molecules (e.g. other H_20 molecules in water) through a new kind of bond, a 'hydrogen' bond.

A.3.1.3. Boundary (section 3.3.3.3):

B = <P, I>

P = the combined outer shells of oxygen and hydrogen, the latter exposes an empty slot since it only has one electron in a shell that can hold 2.

I = electrons in each shell are available for further chemical interactions dependent on the other kinds of molecules in the environment. The polar geometry of the molecule allows it to form a new kind of bonding (not covalent or ionic).

A.3.1.4. Transformation(s) with reference to the G interactions above (section 3.3.3.4):

A water molecule is relatively inert since all of the valence electron spaces are occupied. The molecule can participate in hydrogen bonding with (it is thought) four other water molecules which then forms a network of molecules giving water its properties. A water molecule can also participate in various ways with non-water molecules by either positive (hydrogen pole) or negative (oxygen pole) affinities making water molecules instrumental in affecting other chemistries. All possible such other entities would need to be listed in the G set and their interactions with water in the T set.

The water molecule can absorb energy to change its vibrational mode and the electrons in the valence shells are subject to photon influences. In some cases, the effects of other molecule types can influence dissociation into H^+ and OH^- radicals in aqueous environments but this is not a transformation of inputs into outputs unless one considers that the 'molecule' still exists in the sense that the potential for re-bonding still exists.

A.3.1.5. Memory or history (section 3.3.3.5):

Similar to the atomic “memory”.

A.3.1.6. Δt (section 3.3.3.6):

A time constant small enough to capture the dynamics of electron transitions or small enough to capture vibrational mode frequencies.

A.3.1.7. Level 2 – Subsystems of Molecules

The atoms, H2 and O along with their electrons constitute the level 1 subsystems. Relations between the atoms with respect to geometry need to be specified (see Figure A.2 above) in order to establish the polar nature of the molecule. The decomposition of each atom (as in the prior example) constitutes a level 2 analysis (and further decomposition of the protons and neutrons would constitute level 3).

A.3.1.8. Onto/Combo-genesis

Hydrogen and oxygen have high affinities to share electrons. The reaction is exothermic and can proceed with very little external energy input. Indeed, the reaction is explosive unless constrained by control of the rate at which the atoms are brought together. In general, the combining of atoms is governed by the laws of chemistry involving electric charge interactions.

A.3.2. Larger, More Complex Molecules

The range of molecular systems and molecular interaction networks is huge (possibly infinite?) The range is not only in terms of complexity of combinations of atoms, but in terms of size as well. Our examples of very large (macro-) molecules include those needed for living systems, in particular proteins and nucleic acids (DNA and RNA). These molecules are examples of complex systems. Most small molecules are not adaptive in the sense described in Chapter 9, section Adaptivity. However, when we consider the proteins that perform enzymatic actions, we are looking at the beginning abilities for molecules to adapt to dynamically changing environments.

This appendix is not able to provide the kind of descriptions of the systemness of this class of molecules, obviously. But we suspect that a good graduate student project would be to do so for a well-known enzyme molecule!

A.4. Living System

A.4.1. Prokaryote Cell

Our final example in this appendix is from the earliest known life form, a prokaryote cell, a bacterium, for example. A living cell is already orders-of-magnitude more complex than a protein molecule; it is comprised of several hundred molecular species from small metabolites, water, and dissolved salts to a, comparatively speaking, huge strand of DNA that carries the genetic knowledge.

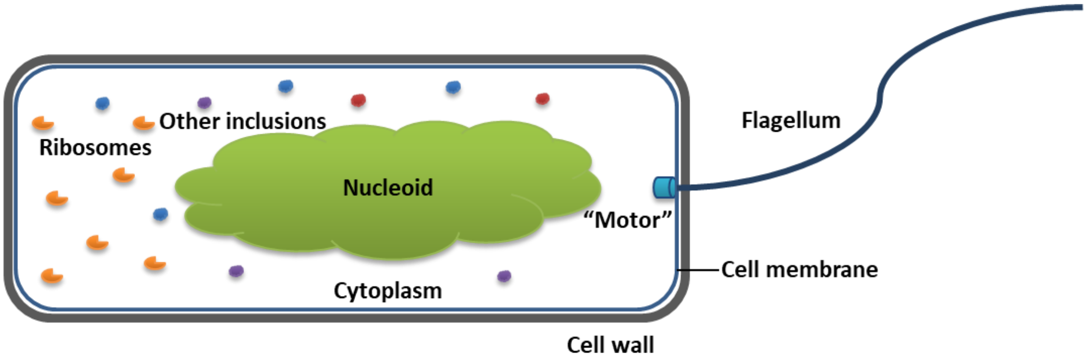

Fig. A.3. A prokaryotic cell and its level 1 subsystems.

A.4.1.1. Components and Internal Network of relations (section 3.3.3.1):

Here we just include a few component subsystems (appearing in Fig. A.3) to show the structure of the framework equations. There are many more components that would show up at level 1 and thus the sets of components and relations would be quite a bit larger than shown here.

C = <{Cyt, 1}, {Nuc, 1}, {Fla, m=species depend}, {Rib^+, 1}, {inclusions, 1}>

Cyt = Cytoplasm, Nuc = Nucleoid, Fla = Flagellum & Motor, Rib^+ = many Ribosomes, and inclusions are a multiplicity of macromolecules and structures used in digestion and synthesis

N = <{Cyt, Nuc}, {Cyt, motor}, {Cyt, Rib+}, {Cyt, inclusions}, {Nuc, Rib+}, {Rib+, inclusions}>

A.4.1.2. Network of interactions with environmental entities (section 3.3.3.2):

A general mechanism for prokaryotes to interact with elements in their environment is engulfing a 'particle' through a process of endocytosis (pinching off a bit of membrane – see below – surrounding the particle for internal processing, e.g. digestion) and expelling wastes by a reverse process called exocytosis (where the membrane capsule fuses with the cell membrane pushing the particle out into the environment where it will be carried away). These processes are effectively also the interfaces for the inflow and outflow of material and energy.

G = <{FM, Cap}, {Cap, Env}, {End, Exo}>
Where:
FM = Food molecules;
Env = Environment;
Cap = internal membrane capsual
End = Endocytosis; Exo = Exocytosis

Of course, cells have many interactions with entities in their environments, especially other prokaryotic cells (same and other species). They will also interact with negative entities such as eukaryotic (single celled and multicellular) predators.

A.4.1.3. Boundary (section 3.3.3.3):

Cell membrane and cell wall.

B = <P, I>
P = lipid bilayer membrane https://en.wikipedia.org/wiki/Cell_membrane and cell wall (when present) https://en.wikipedia.org/wiki/Cell_wall .
I = endocytosis and exocytosis using membrane as described above.

A.4.1.4. Transformation(s) with reference to the G interactions above (section 3.3.3.4):

Metabolism (anabolism and catabolism) using molecules ingested in endocytosis and producing wastes purged through exocytosis

A.4.1.5. Memory or history (section 3.3.3.5):

The genome encoded in the strand of DNA copied during cell division including any non-harmful mutations.

A.4.1.6. Δ*t* (section 3.3.3.6):

Millisecond

A.4.1.7. Onto/Combo-genesis

This is essentially the origin of life problem. While many details remain unresolved the evidence for the development of autocatalytic cycles representing a primitive metabolism involving both polypeptides and nucleic acids driven by the several chemical energy gradients in deep ocean thermal vents along with spontaneously forming lipid containers led to protocells. It is unknown how replication or how the genetic code came to be, though there are theoretical reasons to believe they went through some kind of coevolution (the ribosome is made up of RNA and protein and is intimately involved in protein synthesis). In other words, some form of cooperation between molecular species led to the origin of the first living cells.

A.4.2. Eukaryotic Cells

We’ve only touched the surface of complexity in living systems with the above example of a prokaryotic cell, and then only a few example components and relations. One can readily imagine the complexity in eukaryotic (nucleated) cells. These cells, for example in single celled organisms, are, again, many more orders of magnitude more complex than the prokaryote. But as we have seen in this appendix, are subject to decomposition and capture in a knowledgebase. In many ways, of course, most of the work may have already been done by traditional methods in biology. It is perhaps the case that a team of biologists using this framework could construct a knowledgebase for a ‘typical’ eukaryotic cell and from that generate simulation models.

A.4.2.1. Onto/combo-Genesis

Eukaryotic cells are believed to have originated through a process of endosymbiosis where larger (probably Archaea) prokaryotic cell harbored smaller (probably bacteria) that evolved into organelle.