Bottom-up modelling from the chemistry conjunction: building *information* processing structures that encapsulate the essence of the

complexity of any system

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Introduction

Understanding complexity is problematic for science. Proof is most easily obtained by using replicated, tightly controlled experiments that test only one variable. Such abstractions however lose much of the subtlety of the interactions and feedbacks that occur in the real-world complexity. Or more particularly, the results only apply to a small part of the complexity continuum.

While chaos theory and complexity theory can make the subtlety visible, there is a reduced ability for experimental replication and consequently proof of causation becomes more problematic. There is a gap in our understanding as to how to link the easily testable knowledge of much of science with the insights made visible by chaos and complexity theories.

By contrast, ecologists have to struggle with highly visible complexity knowing that, at some point, it is driven by the underlying science. Grimm, et al., (2005) argued for the use of patterns of similar behaviour and bottom-up modelling to understand this complexity, but noted the absence of a general framework for bottom-up modelling.

Meanwhile in composting Chapman (2008) found a demonstrably imperfect model explained the data with a very high regression coefficient. The imperfection in Chapman's model arose from the desire for a pragmatic formulation; one that was useful rather than precise. It was a surprise to get both usefulness and precision. Attempting to explain this apparent incongruence led to the development of the 'navigation tools', called seamlessness and constraint resolution, as guides to assist building the model (Chapman, 2011). Considering the similarities between Grimm's patterns and Chapman's micro-environments, and that Chapman had built his model upwards from an oxygen-based microbial kinetic pointed to this being evidence for the usefulness of bottom-up modelling.

This paper argues that an analysis which uses bottom-up modelling can **begin** with all the implicit complexity and that where seamlessness is compromised is a good opportunity to identify which detail can be ignored with minimal impact on model precision. In addition, there are two locations within this complexity that are argued to be useful for building bottom-up models. These are locations where several of the contributing elements coalesce:

- Chemistry conjunction where molecules meet microbes, and all analytical systems have a common root.
- Mathematical/ Natural system conjunction where the complexity of shapes in the real-world meet the limited range of mathematical geometries that are available to describe them.

It is further argued that as bottom-up modelling is inherently unbounded, then a decision to encapsulate **only** Nature in the model formulation can be made and this enables a creative interface

between Nature and Human use of Nature. This is a potentially useful attribute for humans to address sustainability questions.

Understanding complex systems

Within Nature there is substantial variability at small scales: consider the micro-electrode studies of the distribution of oxygen in activated sludge floc (Li & Bishop, 2004), biofilms (De La Rosa & Yu, 2005; Horn & Hempel, 1995; Zhang, Fu, & Bishop, 1994), two-phase soil-manure systems (Petersen, Nielsen, & Henriksen, 1993) and soil aggregates (Sexstone, Revsbech, Parkin, & Tiedje, 1985). Attempting to accommodate all of this complexity generates over parameterisation problems in composting models (Hamelers, 2001); making determination of the value of the necessary parameters from experimental evidence problematic. That is, we cannot know the system because we cannot determine the value of the parameters necessary to understand the parts. Similar problems can be expected for any complex system. It is not surprising then that most of the knowledge of these complex systems is either: very specific (being derived by measuring only a narrow part of the system complexity), or net of the overall system (when derived by measurement of the full system behaviour - in effect averaging the contribution of the parts).

In composting, Miller (1992) separated the study of individual populations (autecological studies) from the study of the system (synecological investigations). He noted that: "*Ecological investigations of composting have tended to be autecological or synecological, but rarely integrative of these two conceptual paths*" P.516. The specific knowledge (autecological) has value as it is a part of the full system, but as its context is very narrow it has little relevance to other contexts. A complex system will contain many such contexts consequently we need both approaches to understand the system.

With both of these conceptual paths, much of the complexity is embedded either: outside the experimental context in the autecological studies, or inside the averages that are implicit in any measurement of the system (synecological). That is, they are a form of simplification by abstracting from the full complexity. It follows that it is the initial formulation of the area of interest that locates much of the complexity outside the area of immediate interest, so in a derivational sense the two conceptual paths are mutually incompatible as one excludes the complexity in the other. More particularly, using the results derived from one path is likely to be difficult to use in the other. Indeed, Chapman (2008) found this to be the case in composting where the particle size used in trials is rarely mentioned in the accompanying paper, consequently this data cannot be used to support (or refute) a model which finds size to be a significant parameter - as the particular location in the complexity continuum that the results apply to, cannot be determined. The reluctance to embrace the two conceptual paths noted by Miller is, in part, a structural constraint arising from the initial choice of the area of interest (the beginning assumptions - or more particularly the perceived need to make these beginning assumptions). In addition, the initial choice of the area of interest is set by the researcher, and all those elements which influence them. But the discipline, social, political and/or economic context of the researcher (which influences the choice of the beginning assumptions) seems insufficient to fully explain this reluctance.

Complexity is bewildering, it lacks a clear direction, and there are no obvious 'attachment points' by which we can begin any analysis. Indeed the disciplines of chaos theory and complexity theory did not arise until computer simulations could make *visible* the complex patterns of behaviour inherent in many simple systems. In addition to making the inherent behaviour visible, these visual displays stimulate our interest more than the mathematical formulation that generates them. This would seem to indicate that the difficulty humans have coping with the full complexity is, in part, due to our brain

structure – the way we process information. Bor (2012) argues that we can hold only a few things in our memory at one time, but if we chunk items into groups so that the group represents all the items it contains, we can see more and more concepts simultaneously. From this perspective, the initial choice of area of interest can be seen to neatly divide the full complexity in two: the area of interest and *everything else*. The problem becomes manageable by such a division. Indeed, if the information that is excluded by such a division is not significant then this can be a useful strategy, but this condition of non-significance needs to be met at the formulation stage – if the condition is not met then the trial results will have limited use.

Such divisions have served science well as they have resulted in the derivation of the fundamental laws of Nature that apply to many complex systems. But assuming the same strategy applies in all situations may need to be questioned. Consider a measurement of the degradation rate of a composting particle. The fundamental laws and processes will apply within the particle, but the particle exists in a specific context which includes: oxygen concentration, particle size, particle composition etc. Because of the particle's need for a specific context, then any measurement of a *system* of particles must account for the different context of each particle. Any measurement of a system only applies to that part of the complexity continuum contained within the context; it becomes a modeller's choice as to how to include each particle's context in the system context.

Persig (1991) argues for the importance of the 'first cut' and advocates an initial static/dynamic separation. This would arguably include the insights of complexity theory in the dynamic part of the separation. However, the static component of this division would still have the same difficulty in fully explaining the physical complexity that is discussed here.

But do we need to begin our studies with a 'first cut' (such as the autecological or synecological studies of Miller, or the static/dynamic separation of Persig)? Consider the consequences for human use of science in our technologies if we could **begin** our models without needing to abstract from the full complexity, if *all* the complexity was inherent in the starting assumptions. Such complexity would be unwieldy even if it were solvable, so some of the detail needs to be removed before we can have a useful model. However, Chapman (2009b) has shown that some detail can be ignored without impacting on model precision consequently determining **which** of the detail can be ignored without impacting on the model precision becomes an important consideration.

This question is similar to that experienced in ecology where the complexity arises from the range of plants, micro-organisms, climatic and soils variation. Ecologists struggling with understanding these complex systems have adapted Loehle's (1990) proposal of a 'Medawar zone'. In the ecological version, the Medawar zone is that point in the model complexity where understanding is maximised (Grimm, et al., 2005), in contrast to Loehle's original axes of payoff and difficulty. Grimm et al., argued in favour of bottom-up modelling for these complex systems, but noted "*No general framework for designing, testing, and analyzing bottom-up models has yet been established*".

The author's experience

Meanwhile Chapman (2009a) was struggling to understand why his demonstrably imperfect model was explaining the data with an $r^2 > 0.99$, implying some sort of perfection not inherent in the original derivation. The notion of a Medawar zone, as used by Grimm et al., was an excellent explanation for his conundrum and was enthusiastically embraced. Chapman had begun his model from the 'bottom' as the original intent was to understand odour production potential from compost (this having a positive correlation to the *absence* of oxygen as an electron acceptor). It was necessary to understand the distribution of oxygen in order to find the non-oxygenated parts of the composting particle that

generated most odours. Many constraints to the 'purity' of the model were necessary in order that the useful task (odour production potential) became possible as a model output (Chapman, 2008).

Considering that similar issues arise in both the micro-scale of a composting particle and the macroscale ecology of plants and animals suggests some commonality that transcends scale. Indeed, that a concept (Medawar zone) which is useful in both the composting and ecological contexts was originally conceived as an explanation for creative leaps in the institution of science would seem to have relevance here. The term arose from Sir Peter Medawar's characterisation of science as the 'art of the soluble' (Loehle, 1990). Much of Loehle's paper is about stepping outside our mores, the myriad of mechanisms that stifle creativity, referring at one point to a person "*having an unerring creative instinct for discovering interesting problems that were solvable and for extracting the essence of complex problems so that they became solvable"* P.243. Extracting the essence of complex systems is the task of Grimm's patterns and Chapman's micro-environments.

Needing to adequately describe complex systems also arises in the chemical engineering discipline. Chapter titles such as: fluid-particle reactions and solid-catalyzed reactions (Levenspiel, 1972) give clues as to the complexity of processes occurring in the real-world. Ultimately any formulation has to be tested against the experimental evidence, where the pragmatism/usefulness requirement of the description is summed up by Levenspiel: "*The requirement for a good engineering model is that it be the closest representation of reality which can be treated without too many mathematical complexities*" P.359.

Descriptions of complex systems that are used in human technologies are therefore a balance between describing the complexity of the underlying processes and usefulness. For which the complexity arises from the natural system/mathematical interface, while the useful element arises from human use of the information. We need to have the best possible solution if we are to determine the best possible technology.

As Chapman wanted a useful model, the relevance of detail was first judged against the usefulness criteria. His phrasing for this judgement was: *if knowing something in greater detail was not going to result in a different design of compost toilet, then it could be ignored*. The intention being that the model's roots need to be embedded in the fundamental laws and processes but they only need to be sufficiently embedded to support the structure (a technology in this case). An analogy is a tree in the mountains which has to balance the conflicting growth demands of forming roots or growing taller and catching more sunlight. Grow too tall and the roots have insufficient strength to withstand high winds. The balance becomes one of quantity from the food basket, versus length of life (more particularly the risk of a short life).

The experience of Chapman (2008) where a high regression coefficient resulted from a model structure that began with all the complexity then ignored detail only when the consequences of not including it had been considered, suggests a model structure is possible that, when formulated around a **location** in the multidimensional complexity, will be optimum for its intended tasks. If we must begin with all the complexity, yet need to reduce this complexity to manageable levels in order for it to be useful, then the task becomes that of a decision structure that enables separation of the useful detail from that which is of lesser significance and can be ignored. Some sort of model boundaries by which useful detail is retained inside the bounds while non-essential parts can be moved outside.

However, all the complexity in any system is inherently interconnected so everything is relevant; implying that we cannot just 'cut out' detail as this interconnection will have an impact on the model

output. A methodology that removes unnecessary detail but retains the consequences of the interconnections that lead to/from this unnecessary detail would be ideal. The consequences of the detail need to be retained even if the detail isn't. The emergence of *combined* parameters that retain detail without needing the mathematics is argued to occur in the case of the effect of diffusion of substrate in a composting particle (Chapman, 2009b) and the uneven particle surface (Chapman, 2009c).

Beginning at the chemistry conjunction

Chemistry is the discipline that doesn't need a habitable zone in the universe. It preceded life and provides a platform upon which almost everything exists, literally in the rocks and soils that life rests upon, and scientifically – the branch being explored here. Each atom has a location in the periodic table which is based on the number of electrons in its outer shell. The number of electrons in an atom's outer shell determines the way it associates with other atoms – its chemistry. The periodic table is remarkably good at predicting the properties of atoms. Electron acceptor is used frequently in my writings and is a compound which needs only a few more electrons to fill its outer shell – hence oxygen is 2 electrons short of the full shell of 8; two hydrogen atoms can supply these resulting in a water molecule. Chemistry explains why atoms form molecules and compounds, and why carbon is such a useful atom for Nature to build large complex molecules (as it has 4 atoms in its outer shell so it can bind with itself and achieve a full outer shell of 8). Atomic mass links these chemical properties to a material's physical properties.

All branches of engineering begin with the properties of materials which have a chemical composition from which the useful engineering properties arise (strength, density, reactivity etc). Mass balance laws for example, are based on these properties.

Energy, with its associated discipline, thermodynamics, has a mass equivalent (atoms are a bundle of energy) – the conversion of mass into energy occurs primarily in stars, generating sunlight. Energy can be stored in a chemical form, such as organic material, and supports ecosystems when this organic material moves through the food chain. Potential and kinetic energy arise from a mass's interaction with gravity.

Chemistry explains why organic matter looses weight as composting proceeds - the carbon is lost as a gas: CO_2 , or volatile organics; although some water may be lost by evaporation (but this would require energy). Microbial kinetics is chemistry mediated through microbes.

The underlying chemistry is a very good base to begin any analysis because all the apparently separate disciplines of science meet at their chemical roots. It is a good point to begin bottom-up modelling.

The mathematical/Natural system conjunction

A mathematical geometry describes a shape with a smooth surface. However, Nature's shapes do not have smooth surfaces. A cell membrane may 'appear' to be smooth when viewed under a low powered microscope, but at higher magnifications protein molecules protrude from the surface; the surface is not smooth. Indeed this irregularity is essential for the cells survival as it is the means by which food etc. is transported across the cell wall. Many of life's essential functions need this surface irregularity. Life is a 3-dimensional object with a 2-dimensional surface.

Irregularity also occurs at larger scales than the surface proteins. Cut any organic material with a sharp knife and cells will be cut – their contents will flow out leaving an empty space between the cell walls. Use a blunt knife and additional irregularity will arise from the tearing action of the blunt blade.

Surface irregularity also arises from nature's growth forms such as biofilms and flocs. Individualbased modelling can simulate these irregular surfaces as they arise from the *processes of diffusion*, *reaction and growth* (Kreft, Picioreanu, Wimpenny, & van Loosedrecht, 2001). While these biological shapes can be described from the underlying processes, this descriptive process cannot be easily reversed. We can begin with a shape, such as one that may appear in a 3-D image, and apply maths to this surface, but this is only possible on this particular image. Each image will be unique. That is, the image is limited by its context which is the physical boundaries that 'contain' the image. It would require knowledge of all surfaces in the system to describe any system in this manner.

At larger scales Nature forms a range of shapes, be it a leaf on a tree, the trunk of the tree, or an insect living in the bark of the tree. The number of different shapes that form in Nature greatly exceeds the set of geometrical shapes that are available to describe them and these standard geometries are demonstrably imperfect in **accurately** portraying the surface roughness of Nature. There are therefore fundamental limits to the ability of mathematics to describe Nature that arise from both: the limited range of geometries available to describe Nature's shapes, and the implicit assumption of a smooth surface. Any description will always be an approximation. Using a cylinder to describe a pore (Levenspiel, 1972) or a perfectly smooth sphere to describe a composting particle (Chapman, 2008) could only ever be an approximation.

However, fitting Nature's shapes into one of the geometrical forms has modelling advantages arising from:

- The geometrical shapes arose from mathematics therefore they provide a very convenient access point into the discipline. Use any of these geometrical forms and the entire discipline of mathematics can be used on that geometry.
- Much of Nature's variability can be input as a different value in the parameters that describe the geometrical shape, such as particle diameter when a spherical geometry is applied to composting. Length and diameter in the case of a cylinder. Height, width, and length in the case of a rectangle. In addition, for a system with many shapes, each shape has a particular location in the system with conditions specific to this location that impact on the shape's behaviour. The context that the geometrical shape applies to can therefore be widened to include **all** components of a complex system (albeit with an imprecise fit to each component), in contrast to the use of an image discussed above (where the fit to the component that the image applies to may be precise, but the image is only a single component of a multi-component system).

Using standard shapes has other advantages. For example, separation of the air phase from the solid in composting is easily achieved by thinking of compost as a collection of particles with air in the gaps. A composting particle becomes the model's *analytical boundary* (Chapman, 2008) while the air outside of the analytical boundary is the oxygen transport system. The essential tasks can be separated even if they are in close physical proximity.

It follows that mathematics is very good at describing processes that occur **within** Nature's shapes, but begins to be limited in accurately describing any process which is surface area dependent and becomes highly complex if there are many shapes in a system. For use in improving technologies,

what is needed is a 'sufficient' description that accounts for all the shapes in the system **and** captures the biological performance of each shape without relying on an accurate description of each shape. The arguments advocated in favour of the emergence of **combined** parameters (Chapman, 2009c), if proven, would have considerable value in reconciling this mismatch. Whether the contribution of micro-pores in transferring oxygen from the air to microbes in a composting particle enters the model as a complex set of equations, or the more expedient (albeit technically incorrect) method of using an appropriate value for the diffusion coefficient from a perfectly smooth geometrical surface, ultimately must rest in their respective abilities to explain the evidence – the regression coefficient.

If modelling 'perfection' is not possible, then a way of navigating through the complexity to the 'location' that is best for the purpose, is indicated. Navigation, especially when navigating blind, is best achieved with a set of tools.

Navigation tools for complex systems

Bottom-up modelling is advocated by Grimm et al., (2005) and supported by the experience of Chapman (2008) where this approach resulted in a very high regression with data. The navigation tools assist the building of the model from the bottom.

In the first instance, there will be some broad scale purpose for the investigation, such as Chapman's intention to understand microbial degradation of our faecal waste streams to enable improved technologies. This purpose will identify a set of initial constraints requiring to be met by the model formulation, such as: nature of the material (faeces present different constraints to urine), intended use of the output, need to input climate data etc. Sustainability criteria can also form part of this initial purpose (Chapman, 2015). These initial constraints are sufficient to begin formulation of the model detail. For example, degrading faeces microbiologically will need consideration of the electron acceptor distribution in a particle, where the need for knowing electron acceptor distribution arises from the chemistry of microbial kinetics; and oxygen needs to get from the air to the site of a microbe. The nature of faeces requires consideration of the geometry of the particle; in contrast to the nature of urine.

Building the model from the bottom (the chemistry conjunction) begins with very little complexity – a single substrate with a single electron acceptor and their associated rate constant is sufficient for use of a first-order microbial kinetic. Although this set of conditions will apply to only a small volume of compost at a particular point in time. The complexity in composting begins when diffusion laws are needed to explain the oxygen distribution which in turn is necessary to explain the location of the anoxic and anaerobic rate constants. Invoking diffusion laws brings in particle size, its location in the pile etc. The complexity builds.

Two tools can aid 'navigation through this complexity': seamlessness and constraint resolution (Chapman, 2011). Seamlessness ensures that the underlying causation is preserved in the model. Constraints arise when seamlessness becomes compromised. These constraints need resolution to ensure the underlying causation is preserved. However, these locations also provide an opportunity for detail to be excluded with minimal influence on the model's precision. In having to resolve the constraint, the contribution of each bit of detail can be questioned as to its efficacy within the model. For example, needing to accommodate the microbe's response to electron acceptor distribution (a *specific* electron acceptor is a necessary part of all microbial kinetic formulations) led to two possible solutions in Chapman's formulation:

- an additional equation that described the 'fuzzy' transition between a kinetic dominated by oxygen to one dominated by other electron acceptors, as evidenced by the micro-electrode studies noted above, or use a
- zero-order oxygen consumption kinetic in the diffusion law solution which identifies a point at which oxygen concentrations become zero. This 'point location' then determined the transition without needing an additional equation. This is demonstrably incorrect as the kinetic should have become first-order at low oxygen concentrations and the sharp boundary that arises at this point is not reflected in the experimental evidence (Chapman, 2008).

However, for a system already suffering over-parameterisation problems, the simpler zero-order oxygen consumption kinetic had advantages in its computational simplicity which overrode any loss of precision from accurately determining the transition. If this were not the case the regression coefficient would not have been so high. Note that it is not possible for the researcher to revert to a single electron acceptor option, as the causation (originating with the chemistry being described by the microbial kinetic, and carried via the need to maintain seamlessness) **insists** on both being present (oxygen & all others). That is, the model **structure** requires the microbe's physical location to determine the relevant electron acceptor, but this structure is less demanding about precisely where the transition occurs. Consequently, the method used to decide the transition can be qualitative in nature, as in Chapman's decision to go for simplicity over complexity.

Insights arise here in the source of some of the difficulty matching model complexity to usefulness. Models rely on mathematical descriptions of reality. These mathematical descriptions are derived by observing Nature and describing it as best they can. However, a first-order microbial kinetic is only describing one of the metabolic pathways that are available to micro-organisms. Many micro-organisms will preferentially use oxygen as an electron acceptor, as this yields most energy for growth, but in the absence of oxygen will use nitrates as an electron acceptor – the growth imperative is very strong in Nature. That is, two (or more) separate rate constants are required in the mathematical formulation but only one micro-organism is growing as it will. A more complex microbial kinetic formulation may capture the essence of the micro-organism, but at the expense of losing precision due to over parameterisation in the model of the system. At some point, the separation of these two metabolic pathways by allocating them to separate spatial zones (by using a zero-order oxygen consumption kinetic in diffusion laws) **adequately** represents the observed growth rates even though it may be a poor description of what actually happens.

As seamlessness was used to build the model from the underlying microbial kinetic to its application in a composting particle's context, many constraints needed to be resolved. Several of these (in particular: the temperature effect on the constants in the fundamental laws and the moving oxygen boundary) were resolved by forming physical structures called micro-environments (Chapman, 2008). These being onion-ring type volumes of compost that were at a similar state of degradation. New micro-environments being formed as oxygen penetrated further into the particle. The complexity of the interaction of microbial kinetics with diffusion of oxygen, in the context of the particle reduced to a simple summation: the sum of the composting rate of each micro-environment * its proportionate volume.

In essence, most of the complexity becomes embedded in the *detail* necessary to determine the location and state of each micro-environment. Locating the complexity at this point in the model thereby replicates where the complexity occurs in the real-world; the model's efficacy remains high even with the modelling compromises. It is the **model structure** that substantially contributes to the efficacy of its output. Indeed, the description of the system begins to be determined by the system

itself rather than the perspective of the researcher. Such a start to any formulation therefore begins largely independently from human foibles.

The similarities between Grimm's 'patterns' and Chapman's 'micro-environments' was striking and suggests that resolving constraints as seamlessness becomes compromised, with the formation of formal structures for carrying the underlying causation across a constraint, is likely to apply to the ecological context. The autecological data is necessary to determine the state of each pattern (and its boundaries), and the system (synecological) is a sum of the patterns – both autecological and synecological are implicitly included. Perhaps all complex systems can be viewed as the sum of its parts, where most of the complexity can be located in determining the state of each part.

Building Information Processing Structures to encapsulate the complexity

The bottom-up modelling approach being used here needs to identify some limit for models that begin at the chemistry conjunction. This is the task of an Information Processing Structure (Structure).

The intention of a Structure is to capture the complexity of a system therefore **all** the components need to be embraced. These components arise from a number of areas:

- The system boundaries and the components located within these boundaries.
- The mathematical formulations of the fundamental laws and processes that function within the system boundaries.
- Mechanisms by which all influences from outside the system boundaries are able to express within the Structure; such as using the Arrhenius equation to adjust the value of temperature affected constants between the end of one finite interval and the beginning of the next interval (Chapman, 2008).
- All the components necessary to link these formulations with the system including:
 - Information carrying structures whose task is carrying information between components. For example, in composting the value of VOR carries all the microbial complexity into diffusion laws.
 - Emergent parameters. These arise as a consequence of the *interactions* of the various components. For example, oxygen penetration distance (z) emerges from the interaction of microbial kinetics with diffusion laws.
 - Any organisational forms that have a physical structure (such as Chapman's microenvironments or patterns of Grimm). If these physical structures are determined by using seamless parameters, then they will *contain* all the seamless information inherent in the parameter. For example, if z is determined seamlessly and used to determine a micro-environment's boundaries then the resulting physical structure will contain every influence on z (such as: temperature, solubility of oxygen in water, diffusion coefficient, particle location in the pile etc).

Considering that the fundamental laws and processes are in a mathematical form, and the discipline of mathematics is very good at assembling the various parts, then most of the Structure can have a mathematical form. Indeed, even though patterns may have a physical manifestation, the components that determine the state of the pattern (and its boundaries in the case of a micro-environment) will be primarily mathematical.

While the purpose for the investigation may include the intention to locate the Structure in a technology, bottom-up modelling will initially require only the fundamental laws and processes; the Structure is built from this point. As the building process is inherently unbounded, an end point is needed to call a halt to building increasing complexity into the Structure. A consideration in identifying this end point is that we cannot influence Nature's response, but we can influence the conditions under which she operates. The Structure boundary therefore is a good place to enable separation of Nature's response from human decisions. The question becomes one of considering the *characteristics* of the interface between the Structure and human decision making that maximise the benefit.

In addition, a system with a physical boundary (which is implicit in a technology) will have 'fingers' of human influence that occur throughout the system. Locate a compost pile in a warm micro-site and the temperature influence expresses through the value of all the constants, coefficients etc within the Structure that are affected by temperature. The human/Natural system interaction is complex. Locating the Structure boundary **in** the mathematics on the Nature side, where all these temperature affected parameters are located, gives these 'fingers' of human influence access to their proper influence. In effect there are two boundaries: the physical boundary of the system and the mathematical boundary of the Structure describing Nature that occurs within the system boundary.

Having captured Nature's complexity there is a need to make good use of it. A formal approach to using information processing structures to make sense of the technology systems needed for the case of human faecal and greywater wastes is proposed in Chapman (2013).

Discussion

Beginning at the chemistry conjunction will not necessarily alleviate the difficulty the human mind has in approaching complexity, as it involves 'an initial plunge' into this complexity, albeit the plunge is not without a guide. An alternative approach which retains all the initial complexity, yet satisfies the mind's need for grouping items to make them understandable, can be formulated around an *interaction in a context*.

With this formulation, the context that every analysis occurs within is assumed to be a component of the model and can be either explicit or implicit. The contexts of the fundamental laws and processes will 'pre-exist' any model formulation as they were established early in the history of science. It follows that much of the context of any complex system will pre-exist any model formulation as little can be done without needing the fundamental laws and processes. In addition, some of the context parameters occur in many of the fundamental laws and processes, as illustrated by the constant temperature context for several of the constants, coefficients and parameter values occurring in Chapman's formulation. Indeed, the context of a carbon-based life form could be argued to be the net characteristics of C, H, O, & N that arise from their respective locations in the periodic table. This suggests a degree of commonality within the contexts of all of these formulations, and this commonality precedes a model formulation. Consequently, from the *interaction in a context* perspective, the *context* can be viewed as holding **all** the complexity. Only the components needed to derive a 'solution' need to be made explicit, which involves moving them from the context into the model bounds. However, as each component is made explicit its linkage to its own context remains. As a model 'contains' the contexts of **all** the components that it uses and, as the contexts all occur within the system of interest (and have the degree of commonality discussed above), they could be argued to be interconnected.

The *interaction* occurs between the explicit components of the model, microbial kinetics and diffusion laws in the case of a composting particle.

Of particular interest for this paper is that the *interaction in a context* phrase also applies as the scale is increased. For example, the context of a pile (which is composed of many particles and air space) could be viewed as an interaction between each particle's composting rate and the pile-air oxygen concentration. Widen the scale further by placing the pile in a technology, then the technology becomes the context and the interaction is the pile's particles with the **conditions** that the technology sets (e.g. temperature, oxygen distribution).

Indeed, the technology will exist in the **context** of a social system. The interaction is between the desired social goals, the characteristics of the technology(s) that aim to achieve these goals and the constraints that influence the technological possibilities (materials, cost etc). Indeed science also occurs within the social system context. Neither the formalisation of mathematics, nor measurement with instruments, occurs in Nature.

The notion of context in this sense can be extended all the way to the planet. This being the context in which human social systems (composed of various structures, technologies, institutions etc.) interact with the planet's resources. At this level, the consequences of a particular microbe's response to an electron acceptor in a particle that occurs in a technology, which is only one of several technologies in a social system of which technologies is only a small part, where the social system is only one of many components of the planet's ecology; is not likely to need consideration in a model, but its consequences will occur therefore it must exist in the **context** of the planet. The question is not whether the effect occurs, so much as determining how the consequences can remain in the model even when the detail is removed.

The planetary context therefore includes the contexts of human social systems, technology and Nature. Where the technology context is a sub-set of the human social system context and Nature exists within the sub-set of the technology context (in the case of a technology that utilises biology). However, the interconnections between the contexts mean that the planetary context is implicit in all our technologies whether we consider it or not.

With an *interaction in a context* applying across all scales then any location in the multidimensional complexity can be chosen for analysis. For which the detail needing to be made explicit (moved from the context to within the model bounds) would need careful consideration. That is, all of the contexts exist and remain interconnected but the 'lens' of the particular area of interest will bring into focus only those components that are necessary for the analysis.

If any location in the multidimensional complexity can be chosen, then there is no impediment to beginning the analysis at the top. The analysis can begin with human existence on the planet where the **purpose** of the analysis enables input of those issues that are important for human existence. Sustainability criteria are increasingly clamouring to be heard in modern society and questions of sustainability can have a place in the analysis where the conditions needing to be met by the best possible technology can be identified. These conditions can then influence the development of technologies. Indeed, such a purpose is argued above to be necessary before bottom-up modelling can begin, as the characteristics of the subject of interest need to shape the formulation.

With all the complexity implicit in a planetary context, the use of hierarchies as used by Grimm et al., (2005) is a useful organisational consideration. Hierarchies are a useful holder of context as they contain an implicit notion of sequential order (Chapman, 2011). The context in which the fundamental

laws and processes were derived occurs at a lower hierarchical level to that of the composting particle that Chapman used them in.

The creativity argued above to occur between an information processing structure and human use of this structure can also apply to the context perspective by considering the different components that are involved in the interaction. Indeed, this creativity applies at all hierarchical levels. It follows that each hierarchical level could be optimised, but lower level hierarchies can only be optimised within the context of the higher level hierarchies. Embracing all of the complexity in the starting assumptions enables such notions.

Even the identification of the purpose that identifies the set of initial constraints can also be viewed as in interaction in a context. Begin with all of the complexity and apply each set of constraints at its appropriate level.

Conclusion

Mathematics is internally more precise than its interaction points with Nature. Making useful models of nature using mathematics approaches an art form in that a balance must be struck between the inherent precision of mathematics and the imperfection inherent in maths ability to describe Nature.

Considering that no mathematical formulation of Nature can be precise leads to the question of how to make best use of the descriptive components that are available. This paper focuses on two useful locations in the complexity, the chemistry conjunction and the mathematical/natural system conjunction. Beginning a bottom-up model at the chemistry conjunction implicitly contains all the complexity of any system as this is the common root of all analysis systems. However, this level of complexity is overwhelming and not very useful. Considering that the mathematical/natural system conjunction puts limits on the possible precision of any mathematical model makes the compromises necessary to embrace the most relevant parts of the full complexity easier. In addition, removing excess detail at the locations where seamlessness is compromised is argued to be a good opportunity by which some of the less relevant complexity can be removed. With attention focussed on this location the contribution of each parameter to the model precision can be considered. This consideration can extend to the intended use of the model.

The mathematical formulations of complex systems have no preferred solution. A number of options are available for increasing the model's efficacy. The tension between modelling complexity and usefulness is discussed; where usefulness can include a wide range of socio-economic considerations. In addition, the notion of 'best possible' inherently contains qualitative judgements as to what constitutes best. Chapman could have asked for the 'smelliest' possible design for his toilet. Consequently, some human imposed measure as to what constitutes 'best possible' is required. Shaping the overall model to output a measure that has a strong correlation to this 'best possible' concept is a further mechanism by which a model's efficacy can be improved.

Interaction in a context is a further possible analysis system which is independent of scale yet embraces all of the complexity.

Bibliography

Bor, D. (2012). *The ravenous brain: how the new science of consciousness explains our insatiable search for meaning.* New York: Basic Books.

Chapman, P. D. (2015). *A sustainable sewerage system for Glenorchy*. Retrieved from paulchapman.nz: http://www.paulchapman.nz/papers/A-sustainable-sewerage-system-for-glenorchy.pdf

Chapman, P. D. (2008). *Application of diffusion laws to composting: theory, implications, and experimental testing*. Christchurch: Unpublished doctoral thesis, Lincoln University: Downloadable version at: http://researcharchive.lincoln.ac.nz/dspace/handle/10182/819.

Chapman, P. D. (2009a). *Parameter determination in composting - Part I: The use of overlaying, interdependent sets of equations as a solution to the over parameterization problem.* Retrieved from paulchapman.nz: http://www.paulchapman.nz/papers/parameter-determination-PartI.pdf

Chapman, P. D. (2009b). *Parameter determination in composting - Part II: Incorporating substrate diffusion and substrate solubilisation*. Retrieved from paulchapman.nz: http://www.paulchapman.nz/papers/Parameter-determination-PartII.pdf

Chapman, P. D. (2009c). *Parameter determination in composting - Part III: Analytical boundary*. Retrieved from paulchapman.nz: http://www.paulchapman.nz/papers/Parameter-determination-PartIII.pdf

Chapman, P. D. (2011). Seamlessness as an aid to bottom-up modelling: matching model structure to reality. Retrieved from paulchapman.nz: http://paulchapman.nz/papers/seamlessness2011(V1).pdf

Chapman, P. D. (2011). *The use of context and hierarchies to extend seamlessness into technology choice*. Retrieved from paulchapman.nz: http://www.paulchapman.nz/papers/context&hierarchies-to-extend-seamlessness-into-technologies.pdf

Chapman, P. D. (2013). Using an information processing architecture as an aid to optimising technology choice for faecal wastes and domestic waste water: Part I - Encapsulating Nature. Retrieved from paulchapman.nz: http://www.paulchapman.nz/papers/Using-information-processing-architecture-PartI.pdf

De La Rosa, C., & Yu, T. (2005). Three-dimensional mapping of oxygen distribution in wastewater biofilms using an automation system and microelectrodes. *Environ. Sci. Technol. 39*, 5196-5202.

Grimm, V., Revilla, E., Berger, U., Jeltsch, F., Mooij, W. M., Railsback, S. F., et al. (2005). Patternoriented modeling of agent-based complex systems: lessons from ecology. *Science*, 987-991.

Hamelers, H. V. (2001). A mathematical model for composting kinetics - Unpublished doctoral thesis. Netherlands: Wageningen University.

Horn, H., & Hempel, D. C. (1995). Mass transfer coefficients for an autotrophic and a heterotrophic biofilm system. *Wat. Sci. Tech.* 32, 199-204.

Kreft, J., Picioreanu, C., Wimpenny, J. W., & van Loosedrecht, C. M. (2001). Individual-based modelling in biofilms. *Microbiology 147*, 2897-2812.

Levenspiel, O. (1972). Chemical Reaction Engineering - second ed. New York: John Wiley & Sons.

Li, B., & Bishop, P. L. (2004). Micro-profiles of activated sludge floc deterimined using microelectrodes. *Water Research* 38, 1248-1258.

Loehle, C. (1990). A guide to increased creativity in research - inspiration or perspiration? *BioScience* 40(2), 123-129.

Miller, F. C. (1992). Composting as a process based on the control of ecologically selective factors. In F. Blaine Metting, *Soil microbial ecology: Applications in agricultural and environmental management* (pp. 515-544). New York: Marcel Dekker inc.

Persig. (1991). Lila: an inquiry into morals. USA: Bantam Books.

Petersen, S. O., Nielsen, T. H., & Henriksen, K. (1993). Direct measurements of oxygen microprofiles and distribution of phospholipid-P in a two-phase soil-manure system. *Geoderma 56*, 549-559.

Sexstone, A. J., Revsbech, N. R., Parkin, T. B., & Tiedje, J. M. (1985). Direct measurement of oxygen profiles and denitrification rates in soil aggregates. *Soil Sci. Soc. Am. J.* 49, 645-651.

Zhang, T. C., Fu, Y. C., & Bishop, P. L. (1994). Competition in biofilms. *Wat. Sci. Tech.* 29 (10-11), 263-270.