

CHAPTER 2. COARSE GRAINING AND BUILDING BLOCK HIERARCHIES

From the previous passage about complexity it was clear that the concept of scale has an important role to play in the following discussions. We introduce in this chapter a formalism to define representations at different scales: coarse graining. We will explain what use it has in the description of a complex system's modularity, which is related to its building blocks and the hierarchy behind its construction. The need for deducing the macroscopic properties of a system from its microscopic degrees of freedom, probably one of the most difficult tasks in science at the moment^[16] is emphasised, and simple examples where this is achieved are shown. This relationship between scales will be of relevance when considering the renormalization group techniques in chapter three.

Towards the end of the chapter we review the organization in hierarchies of the components of systems which have it, their representative degrees of freedom, and their involvement in the study of complex systems as an expression of collectivity.

2.1 Coarse graining

In the physical sciences, the degrees of freedom are parameters that specify properties about the state of a system and enable making predictions of its evolution according to the laws of a given model. By *coarse graining* we mean the process of passing from one representation encompassed by the model of a system based on its ‘full number’ of degrees of freedom, to another based on its ‘effective’ degrees of freedom, due to the expected

reduction and simplification posed. The condition of effectiveness requires that coarse graining constitutes not only a sampling that constructs a compact list of degrees of freedom, but that it also chooses and averages them in a manner that allows to obtain significant information about the system in question, particularly about its structure.

In some cases the effective model happens to be an equivalent description of the system originally characterised by the ‘complete’ set of degrees of freedom. Why we choose to ‘coarse-grain’ it is due to how useful one description can be against other when attempting to solve a problem or to draw interpretations. In some cases the reduction involved does not compromise the accuracy of the effective descriptions, and we focus on such cases first.

So what is meant by the utility of a model? First, that it is numerically tractable. For instance, the many-electron problem can be tackled by means of the Born-Oppenheimer approximation to solve the Schrödinger equation of the N -electron wavefunction, but we arrive to an expression which is impossible to solve exactly. Second, and more importantly, it is sought that the model is able to provide a more profound qualitative picture of the properties happening at the scale where observations are made, may they have collective origins from another scaling or not. A model not falling within both criteria is said not to be of use relative to our observation. So, for the problem of the many atoms, the electron density was introduced as a basic variable^[17] which led to the current density functional approach to this problem, leading to major advances on the understanding of the atomic and molecular structures. Hence that point is where coarse graining comes on stage: in the capacity of aggregation which allows systems to be represented at different scales.

The idea of utility and observation is analogous to the question of measurement, as it implies an interaction between the system of interest and a comparing device, both defined within a respective scaling. How meaningful the measurement results, it depends on the

comparative scale at which properties occur: as we can measure the fluctuations posed by Brownian motion on a particle of pollen on the surface of water we do not try to follow its effect on a football floating on a calm pond. To insist on the study of these fluctuations would hardly offer us a deeper insight or provide with major corrections.

It may be noteworthy that frequently it is coarse grained descriptions that are first obtained in science, as they are related to the level or scale of the observations made. Later, microscopic descriptions become available to explain the earlier effective theories.

2.1.1 Two types of coarse graining in physics

The following examples intend to give a glimpse on what is meant by coarse graining and to emphasise the issue of usefulness with respect to ‘real-life’ applications. These examples are idealised but helpful tools, and serve as ‘effective models’ with respect to the more complicated examples they can represent in principle.

The rigid body

A statistical mechanics-oriented model of a solid may represent the interaction between neighbouring particles by harmonic springs, thus a rigid body belongs to the case where the associated constant k is too high for the scale of the energy involved, therefore deformation by strain can be neglected. The assumption of a system wherein every component stays in a fixed position with respect to every other imposes a number of constraints of the type:

$$(\vec{r}_i - \vec{r}_j)^2 - c_{ij}^2 = 0 \quad (1)$$

The rigid body is defined in classical mechanics as the system of particles where the lengths c_{ij} are fixed and do not vary with time. The number of degrees of freedom associated with a rigid body is greatly reduced due to these constraints; it is six in three dimensions: in order to find a particle's position, by specifying its distance to other three non-aligned fixed points rather than to every other across the body is enough. The nine degrees of freedom of these three particles are reduced to six by inspection of the constraints of equation (1)^[18].

A helpful vector, the weighted average of the particles' positions, defines the centre of mass of the body. For a system of constant-mass particles it is found according to

$$\vec{R} = \frac{\sum m_i \vec{r}_i}{\sum m_i} \quad (2.a)$$

If the mass of every particle is the same, say $m_i = M/N = m$, \vec{R} can be found:

$$\vec{R} = \frac{1}{N} \sum_{i=1}^N \vec{r}_i \quad (2.b)$$

From the conditions of constraint given by equation (1), the position of the i-th particle can be determined if its position with respect to a coordinate system centred at \vec{R} is known. We name these vectors \vec{r}'_i , which are constant and analogous to the c_{ij} values.

$$\vec{r}_i = \vec{r}'_i + \vec{R} \quad (3)$$

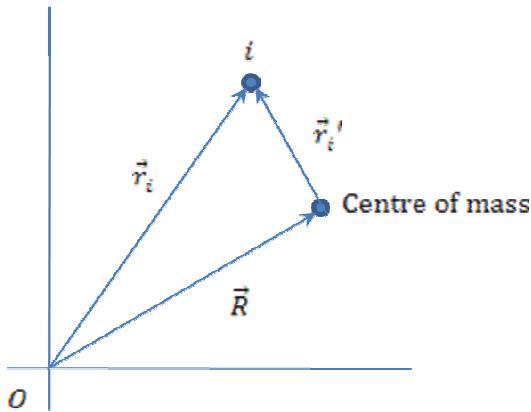


Figure 4. Position of the i -th particle; both in terms of a laboratory coordinate reference system, and the centre of mass reference frame.

Now a description for each of the components' position and motion can be found if all the forces (both external to the body and those due to interactions within the system) acting on every particle are known:

$$\vec{r}_i(t) = \vec{R}(t) + \vec{r}'_i \quad (4)$$

$$\frac{d^2}{dt^2} \sum_i m_i \vec{r}_i = \sum_i \vec{F}_i^{(e)} + \sum_{i \neq j} \vec{F}_{ij} \quad (5)$$

The use of the definition of \vec{R} and Newton's third law of motion^[19] allows one to simplify all the equations of motion for every component to a single one given in terms of the centre of mass:

$$M \frac{d^2 \vec{R}}{dt^2} = \vec{F}^{(e)} \quad (6)$$

With $\vec{F}^{(e)}$ representing the sum of all external forces. For the velocity of the centre of mass, defined $\vec{v} = d\vec{R}/dt$, and under the assumption that no external forces exist, the evolution of \vec{R} is given by:

$$\vec{R}(t) = \vec{v}_0 t + \vec{R}_0 \quad (7)$$

Hence, the motion of every particle at any instant can be known in terms of the initial velocity of the body's centre of mass:

$$\vec{r}_i(t) = \vec{v}_0 t + \vec{R}_0 + \vec{r}'_i \quad (8)$$

Such is the relation between the microscopic degrees of freedom and an effective degree of freedom at a macroscopic scale, \vec{R} . We verify that both dynamics are consistent:

$$\begin{aligned} \vec{R}(t) &= \frac{1}{N} \sum_{i=1}^N \vec{r}_i(t) \\ &= \frac{1}{N} \sum_{i=1}^N (\vec{v}_0 t + \vec{R}_0 + \vec{r}'_i) \\ &= \vec{v}_0 t + \vec{R}_0 \end{aligned} \quad (9)$$

By review of what we have done so far, from equations (2) we have made use of the centre of mass, an averaged measure, which comprises information of the whole body into a single parameter, a coarse graining by itself. The fact that we could write equation (8) in terms of this quantity and some other a priori known constants –equation (3)–, allows us to say the centre of mass constitutes an effective degree of freedom: it represents a configuration of a system with six ‘original’ degrees of freedom.

In the same style effective theories are such in the sense that they describe observables in terms of effective degrees of freedom that represent underlying parameters which have been ‘aggregated’^[16]. In this example, even with the loss of information posed by averaging, the dynamics of the microscopic configurations could still be described due to the conditions of constraint of the rigid body. The antipodal case, the free-particle ideal gas, will now be treated.

The ideal gas

Consider a system composed of $N \sim 10^{23}$ non-interacting particles. A deterministic evolution will be fully characterised by classical mechanics by initially specifying $6N$ degrees of freedom (\vec{r}_i and \vec{p}_i) to be used in the equations of motion; even more, we could attempt to further characterise the microstate by specifying all of the quantum states available. Although the latter varies at a timeframe smaller than that one might probably be interested to observe, the fact that these fluctuations, under the appropriate limits, do not affect the observed macrostate allows us to ignore them so we say these non-interacting atoms behave in fact as point-like particles.

Statistical mechanics gives a less exhausting and more qualitative insight as linking from the micro-states to a macroscopic scale by means of statistical averages. Before its development, the framework proposed by thermodynamics was established where coarse grained degrees of freedom such as temperature, pressure, chemical potentials, etc. were used. A key result found was practically a condensed account of three empirical formulae, the ideal gas law:

$$PV = Nk_B T$$

Thermodynamics' correspondence with statistical mechanics is largely based on the convention that a description of all instantaneous states of a system is pointless as long as they are consistent with respect to a given macroscopic state (likely to be observed); in such case microstates show redundancies, making the use of statistical ensembles instead justified. This constitutes a coarse graining as it relates to a representation associated to properties of a collective origin.

Still, departing from an everything-known description of the microscopic degrees of freedom, the ideal gas law can be derived. For such a system described in terms of positions \vec{r}_i and momenta \vec{p}_i under a heat bath at temperature T , the probability of a j -th microstate with energy ε_j is given by the Boltzmann distribution for the canonical ensemble.

$$P_j = \frac{e^{-\varepsilon_j/k_B T}}{Z} \quad (10)$$

Z is the partition function $Z = \sum_j e^{-\varepsilon_j/k_B T}$ that acts as a normalisation constant as the system is in some microstate. For this function to be determined we need to know the total of microstates available in the whole system. As the measurement of any observable at the macrostate is given as a weighted average² over microstates and their respective probabilities, we say the partition function constitutes another coarse graining in the sense that it sums only over distinguishable states, accounting for the redundancies present in terms of energy.

² Provided all accessible microstates are equally likely, the postulate of equal a priori probabilities holds.

For a system where the only contribution comes from the kinetic energy of the particles $p_i^2/2m$, its sum across all microstates is $\varepsilon_j = \sum_i p_i^2/2m$. We count every possible microstate and then sum. Since (\vec{r}_i, \vec{p}_i) are continuous variables an integration through all the possible states of every particle, $d^3\vec{r}_i d^3\vec{p}_i$ is involved:

$$\begin{aligned} Z(T, V) &= \int \cdots \int d^3\vec{r}_1 d^3\vec{p}_1 \cdots d^3\vec{r}_N d^3\vec{p}_N e^{-\sum_{i=1}^N p_i^2/2mk_B T} \\ &= V^N \int \cdots \int dp_{1x} dp_{1y} dp_{1z} \cdots dp_{Nx} dp_{Ny} dp_{Nz} e^{-\sum_{i=1}^N (p_{ix}^2 + p_{iy}^2 + p_{iz}^2)/2mk_B T} \\ &= V^N \prod_{i=1}^N \int_{-\infty}^{\infty} e^{-p_{ix}^2/2mk_B T} dp_{ix} \int_{-\infty}^{\infty} e^{-p_{iy}^2/2mk_B T} dp_{iy} \int_{-\infty}^{\infty} e^{-p_{iz}^2/2mk_B T} dp_{iz} \end{aligned} \quad (11)$$

By inspection of a formula for the Gaussian integral:

$$\int_{-\infty}^{\infty} e^{-x^2/c^2} dx = |c| \sqrt{\pi}$$

The expression for Z yields:

$$Z = V^N (\pi 2mk_B T)^{3N/2} \quad (12)$$

We can calculate the thermodynamic pressure $P = -\partial F/\partial V$, where $F = -k_B T \ln Z$ is the Helmholtz free energy. Hence for P we have

$$\begin{aligned} P(V, T) &= k_B T \frac{\partial \ln Z}{\partial V} \\ &= Nk_B T \frac{\partial}{\partial V} \left(\ln V + \frac{3}{2} \ln(\pi 2mk_B T) \right) \\ &= Nk_B T / V \end{aligned} \quad (13)$$

So we have arrived to the ideal gas law. Since we have departed from the partition function Z of essentially microscopic origins, the ability to describe properties at the macroscopic scale implies that there exists a collective account of the system which derives in the capacity to elaborate conceptual statements about both observations made at that scale and the underlying model. An approach based exclusively on $6N$ degrees of freedom to study an ideal gas at the empirical scale would hardly lead to explanations for the observations given by Boyle's law for instance. This shows the importance of understanding the emergence of effective degrees of freedom, so it is in this sense that coarse graining may present itself as a tool for the study of systems where collective behaviour and emergent phenomena arise such as some of those we label *complex*. A mathematical formalism of coarse graining will be briefly introduced in the next sub-section.

2.1.2 Mathematics of coarse graining

For a system described microscopically in terms of a vector $\mathbf{X}(t)$ specified by N components (X_1, \dots, X_N) and represented as a point in the configuration space Ω , a coarse graining is defined as a map:

$$\mathcal{R}: \mathbf{X} \rightarrow \mathbf{X}' \tag{14}$$

Such that $\mathbf{X}'(t)$ is specified by N' components $(X'_1, \dots, X'_{N'})$ and represented as a point in the configuration space Ω' . \mathcal{R} also transforms a function G of $\mathbf{X}(t)$:

$$\mathcal{R}: G(\mathbf{X}) \rightarrow G'(\mathbf{X}') \tag{15}$$

Vector $\mathbf{X}'(t)$ can be thought of an effective configuration of the system, containing N' effective degrees of freedom in a space of dimension $|\Omega'| \leq |\Omega|$.

A coarse graining in which $|\Omega'| = |\Omega|$ is said to be a coordinate transformation whilst for that $|\Omega'| < |\Omega|$ is labelled a projection. For the latter we can split the configuration space so $\Omega = \Omega' \oplus \Omega^c$ and note that:

$$\mathcal{R}: \Omega \rightarrow \Omega' \quad (16)$$

$$\mathcal{R}: \Omega^c \rightarrow 0$$

2.1.2.1 Coarse graining as a projection: sets

A simple interpretation of a coarse graining is as a rule that picks specific members of a collection. For the sets X_1, X_2, \dots, X_N the function defined on an element $x = (x_1, x_2, \dots, x_N)$ of their direct product $X_1 \times X_2 \times \dots \times X_N$ which selects its i -indexed component $\pi_i(x) = x_i$ is called the i -th projection map.

A notion of a projection map can be obtained by the introduction of equivalence relations. The equivalence relation $y \sim x$ which associates a particular component y of Ω to another x under a criterion of similarity for some property allows disjoint subsets, namely equivalent classes, to be defined:

$$[x] = \{y \in \Omega | y \sim x\} \quad (17)$$

Any member of the set is a representative of it. The mapping π from an element to its equivalent class is called the canonical projection map:

$$\pi(x) = [x] \quad (18)$$

$$\pi: \Omega \rightarrow \Omega/\sim$$

Where Ω/\sim denotes the quotient set of Ω by the equivalence relation, i.e. the set of equivalent classes. As we recognize such a set represented by an equal or lower number of parameters $|\Omega/\sim| \leq |\Omega|$, we identify the map π with the projection of a coarse graining as in equation (16), hence $\pi: \Omega \rightarrow \Omega'$. By having $x' \in \Omega'$, thus it can be labelled as representative of the equivalent class, i.e. $x' = [x]$.

Interpreting the configuration space as a set of attainable states in which the original system is represented by a point $\mathbf{X}(t)$, its projection to a representative of its equivalent class $\mathbf{X}'(t)$ is a coarse graining. As in this case Ω is partitioned into subsets of cardinality one, an effective configuration space is described by $\Omega' = \Omega/\sim$ accordingly with an a priori defined relation \sim . It naturally proves useful to consider those that uphold the structure of the set of configurations whenever there is one, as the quotient set summarises it.

Counters example 1: Three identical counters are displayed on a three-panel board.

We denote a configuration $\mathbf{X} = X_1 X_2 X_3$ where X_i stands for the number of counters at the i -th panel. For them we define the equivalence relations:

- $X_i = 3 ; X_j = X_k = 0$
 - $X_i = 2 ; X_j = 1 ; X_k = 0$
 - $X_i = X_j = X_k = 1$
- (19)

Associated with these relations is the mapping π between the set of distinguishable configurations on the board $\Omega = \{300, 030, 003, 210, 201, 120, 102, 021, 012, 111\}$ to $\Omega/\sim = \{\{300, \dots, 003\}, \{210, \dots, 012\}, \{111\}\}$. A function of the configuration, its

probability, is denoted as $\phi(\mathbf{X})$. Note that the equivalence relations of equations (19) establish a criterion by size of the largest collection of counters within one single panel.

For the counters being tossed at random the set of probabilities in the configuration space is $P(\Omega) = \left\{\frac{1}{27}, \frac{1}{27}, \frac{1}{27}, \frac{3}{27}, \frac{3}{27}, \frac{3}{27}, \frac{3}{27}, \frac{3}{27}, \frac{3}{27}, \frac{6}{27}\right\}$. As the probability of having a given equivalence class \mathbf{X}' is:

$$\phi(\mathbf{X}') = \sum_{\mathbf{X} \in \mathbf{X}'} \phi(\mathbf{X}) \quad (20)$$

Hence the set of probabilities of equivalent classes is $P(\Omega') = \left\{\frac{1}{9}, \frac{2}{3}, \frac{2}{9}\right\}$.

2.1.2.2 Coarse graining as a projection: matrices

A matrix operator such that $\mathcal{R}^2 = \mathcal{R}$ is said to be a projection operator in linear algebra, since its image remains invariant under the same transformation that lead to it. For the column vector $\mathbf{v} = (v_1, \dots, v_N)^T$ we define a projection operator \mathcal{R} on it:

$$v_i = \sum_j \mathcal{R}_{ij} v_j \quad (21)$$

The elements of \mathcal{R} satisfy:

$$\mathcal{R}_{ij} = [v_i \in [v_j]] \quad (22)$$

Where the outer is the Iverson bracket defined for P , a mathematical statement, as:

$$[P] \equiv \begin{cases} 0; & \text{if } P \text{ is false} \\ 1; & \text{if } P \text{ is true.} \end{cases}$$

In this case for the inner bracket, $[v_j]$ denotes the equivalence class of which v_j is representative. Note that

$$\mathcal{R}^2 = \sum_k \mathcal{R}_{ik} \mathcal{R}_{kj} = \sum_k [v_i \in [v_k]] [v_k \in [v_j]] = \sum_k [v_i \in [v_j]] = \mathcal{R} \quad (23)$$

Counters example 2: The matrix

$$\mathcal{R} = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Complies with the requisite that $\mathcal{R}^2 = \mathcal{R}$ and therefore constitutes a projection operator. Note that by applying this to a vector of univariate functions $\boldsymbol{v} = (\phi(\mathbf{X}_1), \dots, \phi(\mathbf{X}_{|\Omega|}))^T$ of the particular configurations $\mathbf{X}_1, \dots, \mathbf{X}_{|\Omega|}$ as defined at the example above, we obtain $\mathcal{R}\boldsymbol{v} = \boldsymbol{v}' = \left(\frac{1}{9}, 0, 0, \frac{2}{3}, 0, 0, 0, 0, 0, \frac{2}{9}\right)^T$.

It is in terms of a coarse graining that we can identify some structures which we provisionally label building blocks. These are defined in terms of a projective map and appear more or less ‘natural’ to the questions of the problem concerned, just as the selection of a coarse graining is in general liable to an arbitrary selection of which elements to highlight. For instance, other 10×10 projection matrix than the presented above would have returned a different \boldsymbol{v}' that would, however, lack the insight presented in examples at section 2.3.1.

2.2 Building block hierarchies

One of the questions introduced at the beginning was what credit is to be given to the components of a system's performance? Whenever two similar systems are compared, how can their differences overall be attributed to their 'building blocks'?

A formal approach to the term is as a derivate of the J. Holland's "schemata" (Appendix A), which are patterns that identify similarities among information strings, that is, a type of coarse graining. In that sense being able to reduce the information is advantageous when implementing computational techniques, as often required in the study of complex systems. More importantly, as discussed in section 1.1.4, in such study one needs to work with, at least,

- Components that represent information, (i.e. precursors of local dynamics) about structure, individual function, or else.
- Operators associated with interactions (i.e. executors of local dynamics), whose inputs are the previous generators, and that transform them into other type of components (for example collective patterns/structures due to interactions, bound states, etc.).

Hence predicting the overall behaviour of a complex system from its intrinsic structural and functional modularity –and how to extract the latter from the former- is correlated to the detection of those modules of information (their building blocks). A proposed clue is the insight that the contribution from genetic algorithms can offer. Now, as interactions in the

complex systems are often structured it is natural to play with the possibility of an underlying hierarchy in their organization. More interesting is that such hierarchic systems have properties in common, independent to their specific content^[6], which allows their building blocks to be taken to an even more abstract level of study, as required by an implementation of search techniques such as genetic algorithms.

Before introducing them via the *building block hypothesis* of genetic algorithms we will see simple yet illustrative examples about building blocks hierarchies, and their notably quick evolution when compared to similar but non-hierarchical systems.

2.2.1 Stellar nucleosynthesis

An interesting process showing aggregation and a hierarchy of blocks described solely by physical laws, is in the development of large nuclei by synthesis within massive stars. One of the most massive nuclei naturally occurring as a result of fusion processes in stellar nucleosynthesis is iron. Its most common isotope, iron-56, is commonly generated from the radioactive decay of cobalt-56 which in turns comes from the decay of nickel-56. For the latter to be built, fusing together 28 protons and 28 neutrons at a time is physically unlikely, if not impossible. However, the evolution of the stellar environments –ultimately operated by the laws of physics- may allow producing it by fusing lower order composite particles together, which will later be the building blocks for the next element. A possible route for ^{56}Ni nuclei to be fused is shown in figure 5.

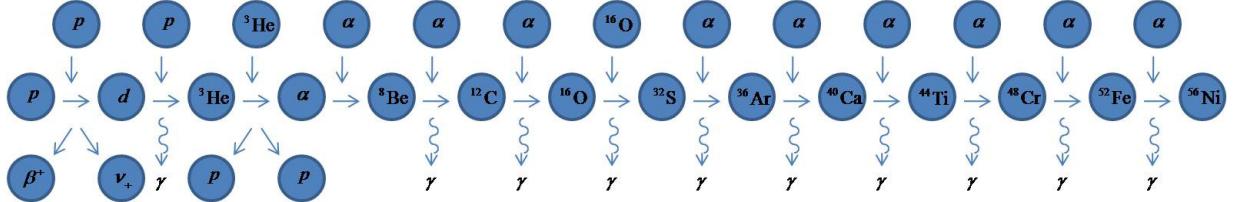


Figure 5. One possible path to assemble the ^{56}Ni nuclide from its ‘primary’ building blocks, protons (for a more complete list, see Appendix B).

From the point of view of the nuclear reactions involved, each step of the sequence depends on the environmental conditions, particularly temperature and density. In addition, the nature of the rules governing nuclear interactions altogether impose boundaries on which reactions are promoted, and which will be less common, rare, or nonexistent. However, to describe the chemical evolution, local properties, namely the cross sections of the lesser order particles and their abundance –governed by the composition of the star (metallicity, fuel exhaustion) and internal structure (e.g. of density distribution, of mass and energy fluxes); need to be taken into account. Woosley *et al.* put nucleosynthesis (in the pre-explosive state of the star) as a function of at least: a) the evolution of the mass of the star, b) its initial composition, c) the set of nuclear physics employed in its study, d) the treatment of convection^[20].

Instead of using closed analytical expressions for about 4,600 bound nuclei from hydrogen to lead^[21], it is more adequate to follow chemical evolution in stellar nucleosynthesis with nuclear reaction networks^[22] which synthesise the corresponding modelling nuclear reaction differential rate equations between parent and daughter nuclides and vice versa as coupled, linearised arrays^[22,23].

As a result of different rates, the production of nuclei is not uniform across elements for different models of stars^[22,24]. The stability of the nuclides plays a role in this effect. In figure 5 some of the elements in the chain are unstable; as long as they achieve to fuse with the relevant particle in due time, the information they portray is maintained, from which another particle is built up. The preferred direction is towards larger, more tightly bound stable nuclei as the inherent loss of energy of the star causes less of it to be available to form excited, unstable or smaller nuclei (via photodisintegration, for instance). Even though such reactions happen, they tend to cost energy, and the inverse is favoured as the star conditions promote exothermic reactions.

An interesting feature of nuclei stability is that of a ‘natural selection’ analogy applied to the sequences of nucleosynthesis^[16]. Nuclear fusion reactions up to iron-56 ordinarily involve mass conversion to released energy, with the mass difference being the nuclear binding energy which is generally higher for an increasing atomic mass (see Appendix C). In the spirit of identifying the decrease of the energy stored in the nucleus with a ‘fitter’ configuration (i.e. less likely to be modified by either radioactive decay, disintegration or fusion with other nucleus) we can apply the notion of a fitness landscape^[16], related to the four variables aforementioned. This landscape shall be subject to the different degrees of ‘preference’ in the interaction (or sequences of interactions) involved, and illustrates the presence of some tightly linked reactions; such can be identified with epistasis, the expression of differences in phenotypes due to genes’ degrees of influence over others, in the language of population genetics.

The concept is inspired by the idea from evolutionary biology of a function which assigns a fitness value (a scalar) to a particular configuration (originally genotypes, generalised to

solutions in evolutionary optimization) of N –an arbitrary number of- degrees of freedom. It is noteworthy that research in complex systems has led to modeling of evolutionary dynamics as many-body dynamics under energy landscapes^[25]. Whenever this function can be determined, the $N + 1$ -dimensional plot of the fitness function defines a surface spanning the space of configurations, hence the term landscape. In this example we may identify the average nuclear binding energy with a fitness function, as it corresponds to a lower potential energy. Under this criterion a more successful nuclide will be that nearing the saturation region centred on the iron-nickel stable isotopes, as overall the evolution suggests a selective pressure towards these elements. Also note that such fitness function depends on the evolution of the host star, which partially depends itself on the processes of nucleosynthesis taking place; a picture of co-evolution.

Although the analogy needs to detail what the fitness function is (which corresponds better to models of nuclear structure); it may help in clarifying the likely path of the evolution for a set of initial nuclei by means of the tools of evolutionary algorithms. Mutation operators could be associated to decay modes of the lower order blocks (namely subatomic particles), or, in a more elaborate way, to the aggregation processes of the higher order atoms; hereafter selective operators tend to prompt a drift of the initial configuration towards local maxima (or minima, depending on the interpretation fitness/potential) of the landscape. It would be interesting to compare these results with the observed pre-supernova isotope abundances.

For an example of a fitness landscape, we show one related to stability of the transuranic elements in figure 6. In this case the configurations space is not the binding energy but the ratio of protons to neutrons in the nucleus as it is decisive in the balance of electrostatic

repulsion and nuclear force attraction of the larger nuclei. The fitness measure is given by the respective nuclide half-life.

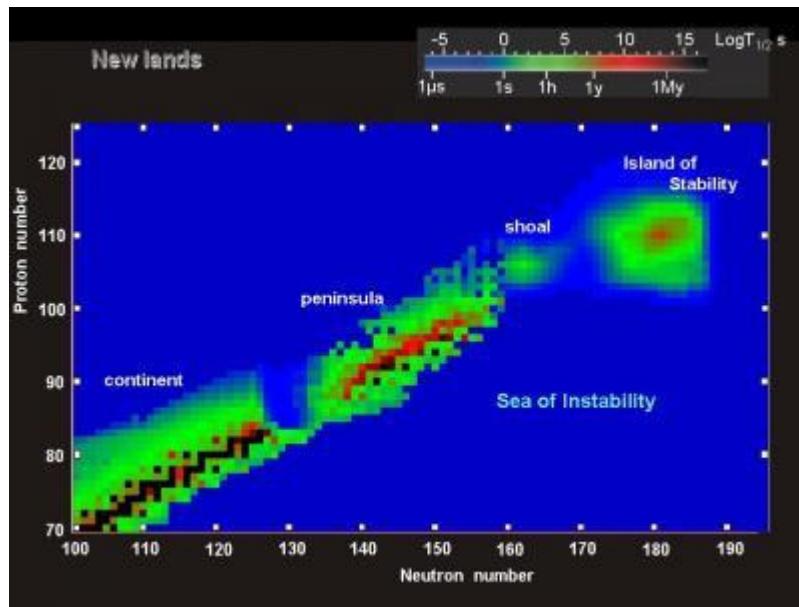


Figure 6. The ‘island of stability’, a proposed region of configurations for super-heavy nuclides which could have a relatively long half-life, in a fitness landscape for the transuranic elements. For instance, element 114 has been successfully synthesised and is relatively stable when compared to other nuclides^[d].

Later on we try to show quantitatively the benefit of clustering by partial aggregation for evolution.

2.2.2 Characteristic scales in biology

It was mentioned earlier in the examples about the structural organization of matter that building blocks could ‘coexist’ in a range of scales determined by energy and remain largely independent of events at other scales. Whenever such clear-cut definitions of energy

ranges become less clear, the scales involved turn less ‘characteristic’ thus leading to other interesting phenomenological descriptions (for example in the aggregation of vortices at different levels of scale in a fluid flow simulation^[26]).

This case is more frequent in the levels of organization in biology. The difference with most physical systems is that as the characteristic scales lose definition, the influence a block has onto the following level in the hierarchy cannot be neglected. It seems that biological systems develop from a point where characteristic scales of energy overlap and the capacities to describe them in reducible frameworks are blurred. That the characteristic levels in biological systems are overlapped means there is more place for subtler phenomena to have a noticeable effect at an unprecedented scale. However the increased sensitivity to initial conditions does not lead to chaos across the biologically-related complex systems. Pervasive to these is the presence and use of fitness, strategies and adaptation, which may be the inducers of interactions between blocks across different levels^[27].

Emerging properties such as those due to aggregation (shape and density for instance); and others closely related to interactions (cycles³, chemical pathways, networks, movement) add more resources to the general panorama for these complex systems to evolve. They do in a different way from the aimless chemical evolution, as the feature of adaptation is central to the evolutionary biology processes, which served as inspiration of evolutionary computation. Reciprocally, evolutionary computation presents with a formalism to the study of evolutionary biology processes.

³ In this sense the carbon-nitrogen-oxygen cycle is an emergent feature of nucleosynthesis in some stars.

2.2.3 The building block hypothesis.

We have already presented some examples where ‘building blocks’ as a qualitative construction seem evident to intuition, but still need to encompass them into a formal definition. It was mentioned earlier that evolutionary computation via genetic algorithms would offer a kind of formalism taken from the study of the performance of genetic algorithms themselves. From their most important theoretical justification^[28], the “building block hypothesis”, we find a quantitative framework for use in the following sections.

We begin by considering a system whose state can be represented in terms of a space of distinguishable attributes encoded in one-dimensional bit strings, the set of possible values in a binary string is $V_i = \{0,1\}$, and we assign an asterisk as the “don’t care” symbol. A schema of six attributes defined on positions 1,2 and 4 is shown on figure 7.

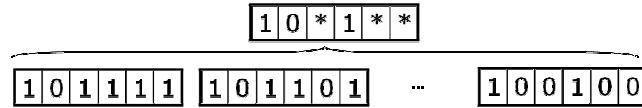


Figure 7. Schemata of bit strings. The notation here has changed from the *don’t care* square to an *.

In evolutionary computation, a fitness function assigns each string a value which characterises its ‘goodness’ as a solution to a specific problem of optimization. For a schema this is evaluated as the average of their component strings.

The *building block hypothesis* refers to the description, under evolutionary algorithms, of the adaptive mechanism of a system through achieving high fitness schemata. It states that by starting with low-order schemata which have a higher-than-average fitness, a genetic

algorithm works by juxtaposing them onto higher order, even fitter schemata. The benefit of these type of schemata, namely the building blocks, is that it reduces the problem's complexity: instead of having high fitness strings built from scratch by trial and error, already known best partial solutions serve to construct even better strings^[29].

Holland schema theorem states that schemata which are defined in a longer range of bits have a higher probability to be destroyed when the genetic algorithm dictating its evolution performs crossover (i.e. one-point recombination: a point in the string is selected so all data from it belongs from one parent string, while the rest is the other parent, see figure 8). Its formulation is:

$$\langle \phi_\xi(t+1) \rangle \geq \frac{f(\xi,t)}{\bar{f}(t)} \left(1 - p_c \frac{\delta(\xi)}{l-1} P_{diff}(\xi) \right) (1 - p_m)^{o(\xi)} \phi_\xi(t) \quad (24)$$

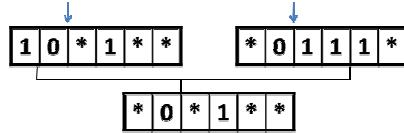


Figure 8. Crossover for the schema of figure 7 with another schema. The crossover point is indicated by the arrows, and the parent schema shares now two attributes from the first parent and four from the second.

That is, the expectation value of the number of strings associated to schema ξ at time $t + 1$, has a lower bound when considering the possibilities of schema disruption due to proportional selection, single-point crossover and mutation of the schema of length l at a time earlier. For the contribution of proportional selection, $f(\xi, t)$ is the time-dependent mean fitness of the individuals in the schema, which is normalised by $\bar{f}(t)$, the mean fitness of the total population. The part due by recombination is just the probability that the

schema survives it: p_c is the probability that crossover occurs, $\delta(\xi)$ is the defining length of the schema (the distance between the first and last attributes other than “*”, as schemata defined in more attributes are more likely to be destroyed), and $P_{diff}(\xi)$ is the probability that parent schemata introduce changes to schema ξ . The last contribution is from the probability of not changing an attribute of the schema; p_m is the probability of mutation and $o(\xi)$ is the order of the schema.

In this sense the term *building block* relates to the idea of shorter, lower order schemata being the most likely to be preserved when under the operators of a genetic algorithm.

However the building block hypothesis does not precise how long a schema should be or, what is the fitness associated to it. Also, the limitations of an equation on schema evolution (the motivation for Holland schemata theorem) are that, at most, they indicate how to build higher order schemata. The valuable outcome from both is the potential to find a hierarchy based on these schemata, associated to the intuition of their evolution given by the building block hypothesis, which will be noticed from the examples of this chapter and in chapter four.

Note that fitter schemata should survive crossover. In population genetics it is often the case of epistatic linkages: interactions between genes which effect their traits in a coupled manner, usually in cooperation towards increasing fitness. For schemata, if they exhibit a higher fitness due to linkages, that means there is a contribution to fitness which is location-dependent, which raises questions about the decomposability of the related fitness functions. A fitness function which exhibits a number of units whose configurations are

highly correlated among each other within the unit but not to configurations in other units, is said to consist of a number of landscape blocks^[16].

In this case a good search algorithm involves recognition of such linkage patterns: considering the building block hypothesis it is necessary to have a representation which places these landscape blocks as close as possible in the configuration space, thus making them compatible with building blocks schemata.

In previous examples of coarse graining we have seen other type of schemata, seemingly less related to the question of *how do genetic algorithms work*. Relating them to the more formal building blocks of evolutionary computation just showed involves the question of representation, and in genetic algorithms these have been traditionally based on binary strings^[29,2].

2.3 Why building block hierarchies?

An observation about complex systems can be inferred from the fact that their subsystems possess information that influences in a non-trivial manner the information correspondent to the “whole” effective system. It can be also observed that not all particular problems are required to exhibit building blocks and that the question is related to whether the system is nearly decomposable^[16].

2.3.1 The watchmaker analogy

This is a parable on the evolution of complex systems by H. Simon^[6]. He presents it with the story of two watchmakers, “Hora and Tempus, who manufactured very fine watches. Both of them were highly regarded, and the phones in their workshops rang frequently - new customers were constantly calling them. However, Hora prospered, while Tempus became poorer and poorer and finally lost his shop.” He explains the cause of frustration being customers’ calls which would interrupt the watchmakers assembling work, thus destroying all the advances made so far.

The main difference is in the approach each one has in the manufacture of their goal: to bind together a thousand pieces of a watch. Whilst Tempus initiates his work from piece one, attaches piece two so on and so forth until finally assembling piece number one thousand into his watch; Hora would work in subassemblies, by first building ten groups of ten pieces each, which would constitute the subassemblies of other ten similar subassemblies, which would shape a completed watch.

The quantitative analysis Simon suggests to explain the different fate of both watchmakers is by means of the probability p to receive a call during the assembling process, and it goes as follows: for Tempus, the probability to finish a watch as one single assembly from start to end is $q = (1 - p)^{1000}$; for Hora, to accomplish one of the 111 assemblies it takes to build the whole watch, he has a probability of $q = (1 - p)^{10}$. Interrupting Tempus means losing the time invested in assembling $1/p$ components on average (if p is smaller than 0.001 then he can normally produce a complete watch on one single go); as *any* call from

Hora's phone will, on average, consume the time destined to bind five subcomponents at any scale.

The average time lost before an assembly can be completed depends on the average time consumed per attempt failed, $\bar{\tau}_{waste}$, this we multiply by the total number of attempts made and divide by the number of those that are successful. The latter proportion is just the inverse of the probability to finish one assembly without interruption, q^{-1} . So, in order to know the average time spent in the overall construction of a watch, \bar{T} , we need to multiply by the number of goal assemblies, N_{sets} : only one in Tempus' case and 111 for Hora's. We have:

$$\bar{T} = N_{sets} \bar{\tau}_{waste} q^{-1} \quad (25)$$

We can attain a more general overview on the benefits of a “constructive” approach by hierarchies compared to the linear assembling of a system of many components, if we study the proposed ratio in the parameter space of both the number of components, stable levels and components per level (leading to a grasp on what N_{sets} and $\bar{\tau}_{waste}$ are); and the probability p .

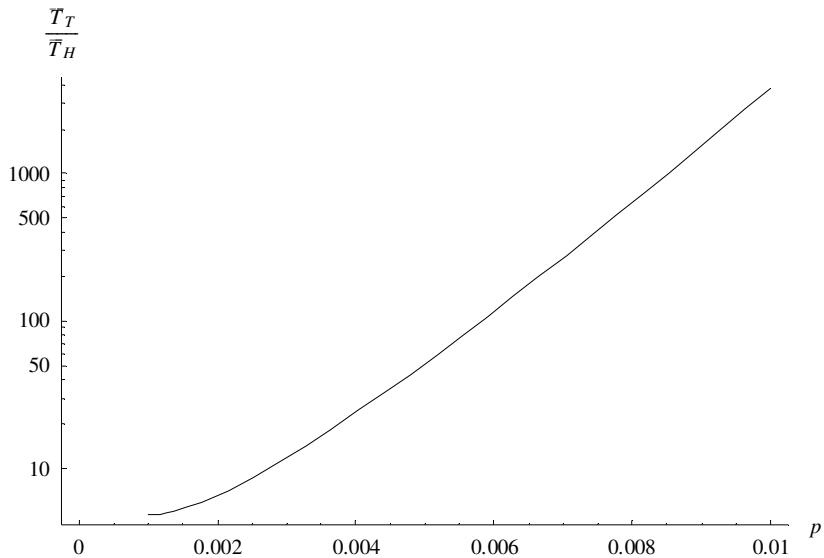


Figure 9. Simon’s line of argument for the proportion \bar{T}_T/\bar{T}_H in a scenario with probabilities smaller than 0.01. There is a minimum in the plot, when p is 1/991, yet there Hora’s approach shows to be at least more than four times as quicker as Tempus’. Larger probabilities of interruption add an exponential growth in the relative time it takes for both watchmakers to finish.

The ratio of average number of times taken to accomplish a watch in the presented scenario is always superior (in advantage) when a hierarchical tactic to build is used. Simon presents this proportion when $p = 0.01$, and it can be calculated that the duration it takes Tempus to finish is almost 3,800 times longer than it takes Hora, leading to no actual competition for the smarter watchmaker.

Now we try to extend some of the ideas about evolution with a thought experiment. We consider a system of free particles/units that achieve a binding/assembling interaction whenever they are “near enough”, i.e. they are both located in a same “partition” of a region which satisfies the conditions for cohesion to occur. The motivation for this is the potential relation to nucleosynthetic processes, the watchmakers example on the quickness of evolution via partial assembling, and the analogy to previous work on coagulation as

evolution of clusters concentration which aggregate irreversibly, namely the Smoluchowski equation^[30].

The volume of the partition can be defined on the basis of the units' properties (e.g. the minimum energy in the potential of interaction). The probabilities for these new states to be formed shall be described accordingly to the characteristics of the particular systems being modelled, such as the number and distribution of composing units, the nature of the interaction, etc. For systems that involve higher densities regimes it is plausible that the number of units is comparable to the number of partitions so there are significant chances for units to encounter one another.

We build a region of reference divided into compartments for which units may be present or not, the volume of the former defined by the rule that any N particles sharing the same compartment at the same time lapse will form an upper bound-state altogether (in other words, it is the maximal extension of space occupied between N units that still allows combination). Assume groups of $M \geq N$ units constantly redistributing within the region at regular time steps, their spatial distribution given at random and independent of previous distributions. As suggested before, we consider the case where the number of units within our region is constant in time and similar to the number of partitions available, M .

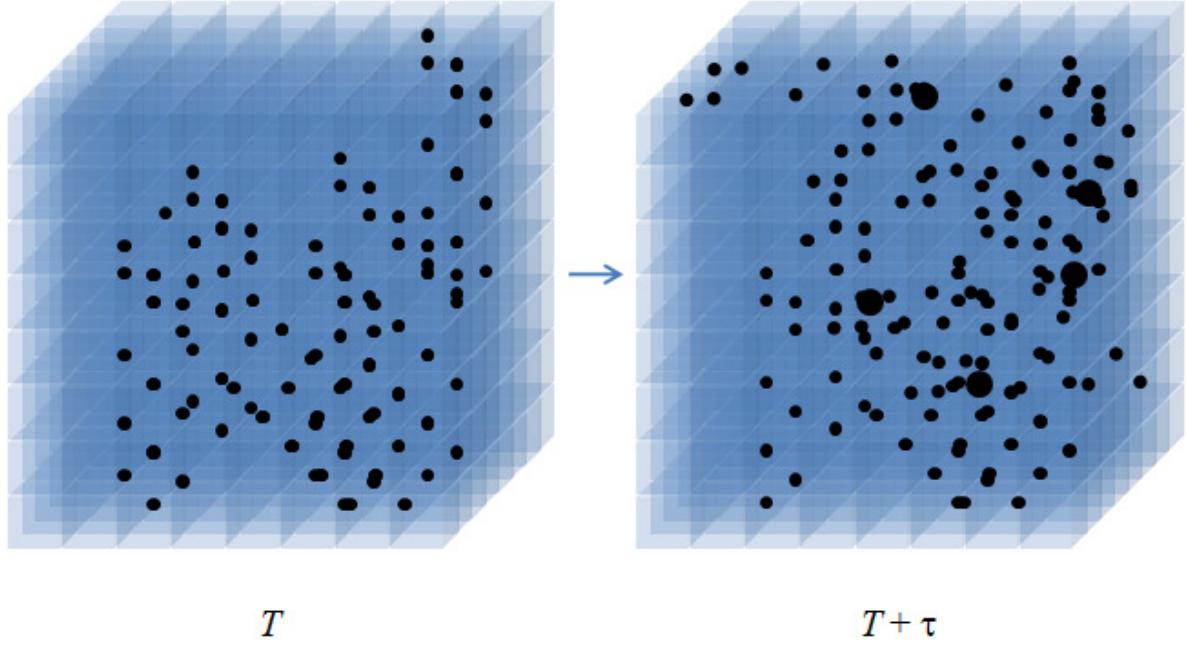


Figure 10. Interpretation of a hypothetical interaction-allowed reference region as spanning a volume wherein a number of units are randomly re-distributed at time steps, enabling new bonds with other single units.

Note that once a bound state has been created, it is assumed stable and non-interacting with any lower-level units. Also, for the moment we will assume that any number of particles in the same compartment that is less than N will not form a bound state (see figure 11). As free particles still, we may interpret this as they are able to follow their mechanical paths and enter other compartments at a later stage.

If the length of our time steps is $\tau = 1$, a particle's location x_i in the i-th box is prone to random change to another within a time step:

$$x_{i,\alpha}(T) \rightarrow x_{j,\alpha}(T + 1) \quad (26)$$

In this sense we can consider the probability for a new distribution given in terms of the previous distribution only. For a random distribution, the probability for a particle to be at a certain time a given partition is $P_{i \rightarrow j, \alpha} = \frac{1}{M}$; $\forall \alpha, i, j$. The expectation value of the number n of bound states formed in this manner at a number T of time steps is:

$$\langle n \rangle = \left(\frac{1}{M}\right)^N T \quad (27)$$

Consider the following, based on the counters example of section 2.1.2. For random rearrangements of three indistinguishable units in three partitions, we may arrive at any configuration out of the ten allowed. Thus we obtain a bound state only when three of them converge at the same time.

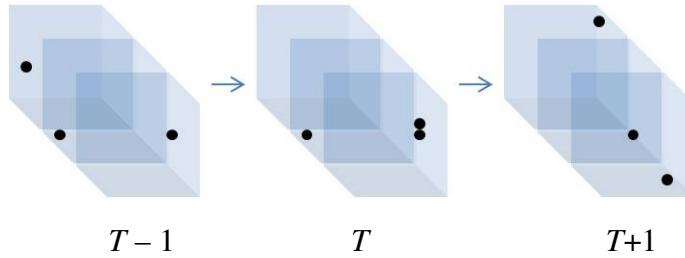


Figure 11. A possible path of realizations under the condition that only N components shall make an assembly by joining each other at the same time T .

We review an example with $M = N = 3$. A Markov chain is characteristic of the process as the probability $\phi'_{x'y'z'}$ to find configuration $x'y'z'$ arises from the probability ϕ_{xyz} of the former configuration xyz times the conditional probability that given xyz , $x'y'z'$ will be achieved:

$$\phi'_{x'y'z'} = P(x'y'z'|xyz)\phi_{xyz} \quad (28)$$

Which complies with the Markov property. Conditional probabilities serve to build the entries of a matrix \mathcal{M} for the transformation at time T to one step later:

$$\begin{pmatrix} \phi_{300} \\ \phi_{030} \\ \phi_{003} \\ \phi_{210} \\ \phi_{201} \\ \phi_{120} \\ \phi_{102} \\ \phi_{021} \\ \phi_{012} \\ \phi_{111} \end{pmatrix}_{T+1} = \frac{1}{27} \begin{pmatrix} 9 & 9 & 9 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 9 & 9 & 9 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 9 & 9 & 9 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 3 & 3 & 3 & 3 & 3 & 3 & 3 \\ 0 & 0 & 0 & 3 & 3 & 3 & 3 & 3 & 3 & 3 \\ 0 & 0 & 0 & 3 & 3 & 3 & 3 & 3 & 3 & 3 \\ 0 & 0 & 0 & 3 & 3 & 3 & 3 & 3 & 3 & 3 \\ 0 & 0 & 0 & 3 & 3 & 3 & 3 & 3 & 3 & 3 \\ 0 & 0 & 0 & 6 & 6 & 6 & 6 & 6 & 6 & 6 \end{pmatrix} \begin{pmatrix} \phi_{300} \\ \phi_{030} \\ \phi_{003} \\ \phi_{210} \\ \phi_{201} \\ \phi_{120} \\ \phi_{102} \\ \phi_{021} \\ \phi_{012} \\ \phi_{111} \end{pmatrix}_T \quad (29)$$

Note that there exists a more ‘microscopic’ version to this transformation if we consider the case of distinguishable particles, leading to an even finer grained description.

For a vector of univariate functions of probability $\boldsymbol{\phi}$, the evolution equation is:

$$\boldsymbol{\phi}'(T+1) = \mathcal{M}\boldsymbol{\phi}(T) \quad (30)$$

Or, for a given initial condition $\boldsymbol{\phi}(0) = \boldsymbol{\phi}_0$:

$$\boldsymbol{\phi}'(T) = \mathcal{M}^T \boldsymbol{\phi}_0 \quad (31)$$

For the evolution of a given configuration we need to know the entries of \mathcal{M}^T and sum over all possible sources in $\boldsymbol{\phi}$ that can lead to that particular configuration in $\boldsymbol{\phi}'$:

$$\phi'(i, T) = \sum_j \mathcal{M}_{ij}^T \phi(j, 0) \quad (32)$$

It can be seen from equation (29) that configurations xyz under the equivalence relations (19) presented before have exactly the same evolution expressions, thus it will serve to use a coarse-grained representation (on position) of the system:

$$\begin{pmatrix} \phi_3 \\ \phi_2 \\ \phi_1 \end{pmatrix}_{T+1} = \begin{pmatrix} 1 & 1/9 & 1/9 \\ 0 & 2/3 & 2/3 \\ 0 & 2/9 & 2/9 \end{pmatrix} \begin{pmatrix} \phi_3 \\ \phi_2 \\ \phi_1 \end{pmatrix}_T \quad (33)$$

Now we will consider a slightly different case where bound states may be achieved by partial aggregation, that is by forming sub-states composed of $N - k$, $k \in [1, N - 1]$ units at possibly different time steps. Here, particles may gather in subassemblies within the region as they constitute genuine stable sub-states.

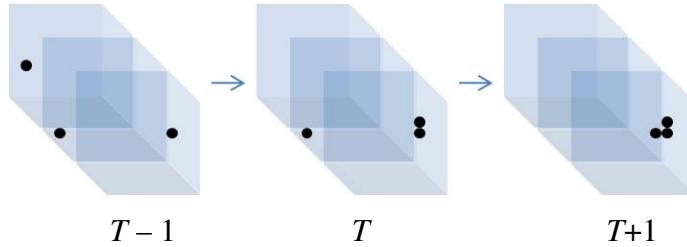


Figure 12. A possible path of realizations under the condition that $N - k$ components shall make an assembly by joining each other at the same time T .

The evolution of configurations probabilities for the $N = M = 3$ case is now:

$$\begin{pmatrix} \phi_{300} \\ \phi_{030} \\ \phi_{003} \\ \phi_{210} \\ \phi_{201} \\ \phi_{120} \\ \phi_{102} \\ \phi_{021} \\ \phi_{012} \\ \phi_{111} \end{pmatrix}_{T+1} = \frac{1}{27} \begin{pmatrix} 9 & 9 & 9 & 3 & 3 & 3 & 3 & 3 & 3 & 1 \\ 9 & 9 & 9 & 3 & 3 & 3 & 3 & 3 & 3 & 1 \\ 9 & 9 & 9 & 3 & 3 & 3 & 3 & 3 & 3 & 1 \\ 0 & 0 & 0 & 3 & 3 & 3 & 3 & 3 & 3 & 3 \\ 0 & 0 & 0 & 3 & 3 & 3 & 3 & 3 & 3 & 3 \\ 0 & 0 & 0 & 3 & 3 & 3 & 3 & 3 & 3 & 3 \\ 0 & 0 & 0 & 3 & 3 & 3 & 3 & 3 & 3 & 3 \\ 0 & 0 & 0 & 3 & 3 & 3 & 3 & 3 & 3 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 \end{pmatrix} \begin{pmatrix} \phi_{300} \\ \phi_{030} \\ \phi_{003} \\ \phi_{210} \\ \phi_{201} \\ \phi_{120} \\ \phi_{102} \\ \phi_{021} \\ \phi_{012} \\ \phi_{111} \end{pmatrix}_T \quad (34)$$

Or in a compact form $\boldsymbol{\phi}'(T + 1) = \mathcal{N}\boldsymbol{\phi}(T)$. The same arguments on configurations xyz and their evolution at time steps apply as in the case before. The coarse grained system is then:

$$\begin{pmatrix} \phi_3 \\ \phi_2 \\ \phi_1 \end{pmatrix}_{T+1} = \begin{pmatrix} 1 & 1/3 & 1/9 \\ 0 & 2/3 & 2/3 \\ 0 & 0 & 2/9 \end{pmatrix} \begin{pmatrix} \phi_3 \\ \phi_2 \\ \phi_1 \end{pmatrix}_T \quad (35)$$

Therefore this assembling makes a hierarchical solution available: the general solution for ϕ_1 depends only in its initial value; this allows to introduce it in the expression for ϕ_2 and solve. Solving for ϕ_3 follows from the already known forms of ϕ_2 and ϕ_1 . The triangular form of the matrix means the set of equations is soluble hierarchically:

$$\phi_1(T+1) = \frac{2}{9} \phi_1(T)$$

$$\rightarrow \phi_1(T) = \left(\frac{2}{9}\right)^T \phi_1(0) \quad (36)$$

$$\phi_2(T+1) = \frac{2}{3} \phi_2(T) + \frac{2}{3} \phi_1(T)$$

$$\begin{aligned} \rightarrow \phi_2(T) &= \left(\frac{2}{3}\right)^T \phi_2(0) + \sum_{n=0}^{T-1} \left(\frac{2}{3}\right)^{T-n} \left(\frac{2}{9}\right)^n \phi_1(0) \\ &= \left(\frac{2}{3}\right)^T \phi_2(0) + \frac{3}{2} \left(\left(\frac{2}{3}\right)^T - \left(\frac{2}{9}\right)^T \right) \phi_1(0) \end{aligned} \quad (37)$$

$$\phi_3(T+1) = \phi_3(T) + \frac{1}{3} \phi_2(T) + \frac{1}{9} \phi_1(T)$$

$$\begin{aligned} \rightarrow \phi_3(T) &= \phi_3(0) + \frac{1}{3} \left(\sum_{n=0}^{T-1} \left(\frac{2}{3}\right)^n \right) \phi_2(0) + \frac{1}{2} \left(\sum_{n=0}^{T-1} \left(\left(\frac{2}{3}\right)^n - \frac{7}{9} \left(\frac{2}{9}\right)^n \right) \right) \phi_1(0) \\ &= \phi_3(0) + \frac{1}{2} \left(1 - \left(\frac{2}{3}\right)^T \right) \phi_2(0) - \left(1 + \frac{3}{4} \left(\frac{2}{3}\right)^T - \frac{7}{4} \left(\frac{2}{9}\right)^T \right) \phi_1(0) \end{aligned} \quad (38)$$

The plot of the solutions is:

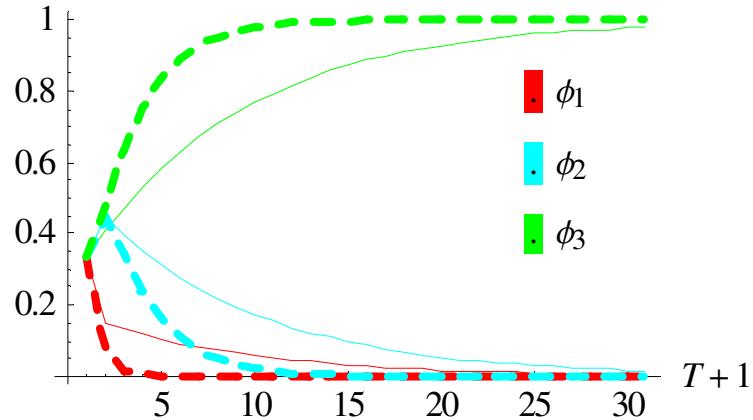


Figure 13. *Even conditions.* Random rearrangements of three indistinguishable units starting with $\phi_1 = \phi_2 = \phi_3 = 1/3$ (ϕ_i denoting the probability of a configuration involving a maximum of i particles at any box at a given time) in the two scenarios: one which will not allow subassemblies (thin lines) and one which does (thick, dashed). After a number of iterations, the fixed points are $\phi_3^* = 1$ and $\phi_2^* = \phi_1^* = 0$. Note that it takes about three times less to saturate the system with 300, 030 or 003 configurations with a subassemblies approach.

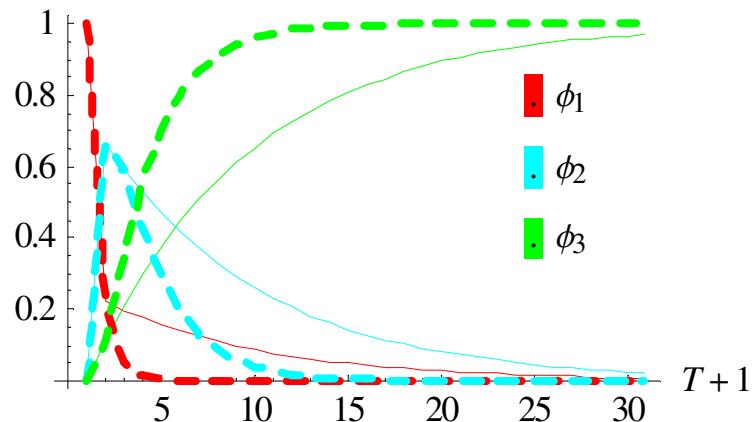


Figure 14. *Building from bottom up.* The same experiment starting at $\phi_1 = 1 ; \phi_2 = \phi_3 = 0$ in the two scenarios.

2.3.2 Modularity

Systems that can be more or less decomposed are said to exhibit modules, component divisions with denser internal connections within, than between one and another. We have implicitly associated this with the idea of a structural hierarchy of modules at different scales: at the macroscopic with effective degrees of freedom reflecting collective excitations of the underlying degrees of freedom inherent to the microscopic scale.

Akin to the idea of the backbone of a complex system being a modular structure, is the consideration of adaptation and the feature of strategies; that is what the effective degrees can “do”, instead of just what they can “be”^[16]. Whenever a number of strategies are to be implemented at a time, by doing so in parallel is usually the most efficient way, which raises the question: as strategies should increase the systems fitness independently what does this effect on the contribution of strategies altogether? It would be interesting to undertake this question in the style of the “structural” building block approach and the quick convergence to an optimum it caused of the last subsection, in the understanding that a higher order strategy is an emergent phenomenon from background sub-strategies.

This kind of behaviour distinguishes the physical from biological systems. In the former there is no place for strategies, associated with functional building blocks. In the perspective of biology, modularity can (and frequently must) be shown in a system’s functions, and relate to their structure.