Self-assembly for supply chains

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**NANYANG
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SINGAPORE

SELF-ASSEMBLY FOR SUPPLY CHAINS

A thesis submitted to the
School of Computer Science and Engineering
at the Nanyang Technological University

by

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Supervisor:

PROF ONG YEW SOON

in partial fulfilment for the requirement for the degree of
Master of Engineering

2019

Statement of Originality

I hereby certify that the work embodied in this thesis is the result of original research, is free of plagiarised materials, and has not been submitted for a higher degree to any other university or institution.

9 December 2019

Date

Gabriel Yee Qi Ming

Supervisor Declaration Statement

I have reviewed the content and the presentation style of this thesis and declare it free of plagiarism and of sufficient grammatical clarity to be examined. To the best of my knowledge, the research and writing are those of the candidate except as acknowledged in the Author Attribution Statement. I confirm that the investigations were conducted in accord with the ethics policies and integrity standards of Nanyang Technological University and that the research data are presented honestly and without prejudice.

9 December 2019

Date

Professor Ong Yew Soon

Authorship Attribution Statement

The thesis contains material from two papers accepted at conferences in which I am listed as an author:

1. **Yee G.**, Ong Y.S., & Tan P.S. (2015) *Emergent Effects from Simple Mechanisms in Supply Chain Models*. In Proceedings of the 18th Asia Pacific Symposium on Intelligent and Evolutionary Systems-Volume 2 (pp. 137-150). Springer International Publishing.

I prepared the manuscript drafts, and the manuscript was revised together with Prof Ong Yew Soon and Dr Tan Puay Siew.

All research was conducted at facilities within the Singapore Institute of Manufacturing Technology and the SIMTech-NTU Joint Lab on Complex Systems.

2. **Yee G.**, Ong Y.S. & Tan P.S. (2016) *Self-assembly of Supplier Selection Strategies*. Paper presented at the 2016 IEEE International Conference on Industrial Engineering and Engineering Management (IEEM)

I prepared the manuscript drafts, and the manuscript was revised together with Prof Ong Yew Soon and Dr Tan Puay Siew.

All research was conducted at facilities within the Singapore Institute of Manufacturing Technology and the SIMTech-NTU Joint Lab on Complex Systems.

9 December 2019

Date

Gabriel Yee Qi Ming

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Abstract

Self-assembly is a natural construction process where components of a system spontaneously form into more complex aggregates when suitable environmental conditions are created. Self-assembly systems are remarkable in that the fabrication of the complex structures are done with mechanisms that are self-reproducing and maintaining, distributed, and are not restricted to having be synchronous. From the perspective of strategy development, such bottom-up behaviours are like the real-world process of systematically identifying and studying the key issues and reasons for a problem before matching it with a strategy to solve it. In a similar fashion, the real-world processes of specifying objectives, tasks, and principles are like the specifying of environmental conditions when designing self-assembly systems. These two behaviours exist as two extreme ends of strategy development causing the typical academic publication on strategy development to dichotomously adopt one. As a science that can bridge both approaches, the ability to self-assemble a strategy would present a superior approach to strategy development.

In this thesis, the conceptualization and implementation of an algorithm that self-assembles a strategy is presented. The algorithm is applied to a supplier selection problem and benchmarked as a symbolic regression solver against traditional Genetic Programming across five representative problems. Finally, the thesis is concluded with statements for potential extension.

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Chapter 1

Introduction

Supply chain management is not a new field. Whilst the term could have been a recent invention (Lummus & Vokurka, 1999; Mentzer et al., 2001), it has been argued, that as a science, it has been practiced since the days of Alexander the Great or as far back as achieving the monumental task of building the pyramids. Since then, the world has become more complex and it has been acknowledged that managing the modern supply chain is a far more difficult task because of the increased amount of information available. Despite the increase in knowledge of supply chain management, it is obvious that more could be done to appreciate and act upon the complexity of the modern-day supply chain. Thus, the purpose for this study would be to create and contribute knowledge that would aid in the management of supply chains through the self-assembly of strategies with the full appreciation of modern-day complexities in supply chains¹².

Even though no works on self-assembly algorithms in supply chain literature have yet been identified, there are many daily activities, other than furniture³, that involve the notion of self-assembly. An example of such an activity would be the development of ideas that, with even further development, become more complicated and complex as they evolve into strategic plans, ranking policies to review partners, or judgement calls. One evidence of this process comes from the study of Synaptogenesis, which understands idea formation or generation to be a result of synapses forming between activated (or agitated) neurons; in other words, ideas emerge when related thoughts are stimulated and linked together. This in a sense, is a form of self-assembly. Like molecular self-assembly which involve simple molecules interacting with each other to self-assemble

¹ For the good reason that it is overwhelmingly laborious and excessively unrewarding, a literature review of Complexity is not included in this thesis. The interested reader is directed to Holland (2014) for a quick introduction to Complexity, and to Mitchell (2009) for a more in-depth study.

² For reviews of Supply Chain Complexity, the interested reader is directed to the works of Choi et al. (2001), Pathak et al. (2007), Serdar-Asan (2012), Surana et al. (2005) and Mariotti (2007).

³ In reference to Ikea's cost-cutting strategy of having customers self-assemble their purchased furniture.

into complex macro-molecules, the eventual product of strategies, policies and reason are the results of thoughts interacting with each other to self-assemble into ideas that go on to become more complicated and complex. The notion of self-assembling strategies for supply chains, the aim of this study, should therefore not be unnatural or alien, but rather be more of a *jamais vu*⁴ and a required understanding for any serious supply chain manager. The challenge of the study is to mimic such mechanisms and then convert them into functional procedures that a computer can perform. By doing so, it becomes possible to reduce or eliminate human involvement and make use of the vastly abundant computing power to autonomously develop strategies for very large and complex supply chain problems.

The attractiveness of self-assembled strategies will come from them being ‘bridges’ between the top-down and bottom-up approaches to strategy development. Top-down approaches to developing strategies for supply chains can be interpreted to be approaches driven by principles (Kotzab, Seuring, Müller, & Reiner, 2006), and with the point of view that the objectives, tasks and principles, when applied, should secure the ‘good’ supply chain. Bottom-up approaches, on the other hand, can be interpreted to be approaches driven by systematic identification of key issues and studies of the underlying reasons for the problem that are then tackled and matched with solutions based on past experiences (Kotzab et al., 2006). Since these two approaches represent the two extreme ends to strategy development, to adopt one approach dichotomously is to not benefit from the advantages of the other. Thus, as a science that is known to bridge both approaches (Whitesides, Kriebel, & Mayers, 2005), self-assembling a strategy could be a superior approach to strategy development.

While full of potential, the self-assembly of supply chain strategies is not a walk in a park; the same difficulties that underlie self-assembly in other fields are also relevant. Such issues include the difficulties in (1) defining precise sets of components and interactions that will result in an appropriate structure for a strategy; (2) ensuring sufficient diversity to avoid local minima; and (3) identifying the relevant information to achieve a functioning self-assembly strategy.

⁴ In French, meaning ‘never seen’. It is a term describing the eeriness experiencing a situation that one recognizes in some fashion, but still seems unfamiliar.

Along with these issues would also be the task of translating the mechanisms that enable successful self-assembly (Whitesides & Boncheva, 2002) from the field of Molecular Self-assembly to Computer Science and Supply Chain Management.

1.1 Research Objective

The objective of this study is to explore the feasibility of self-assembling strategies for use in supply chains. Given the achievements from the field of nanotechnology (Whitesides et al., 2005), it can be expected that these self-assembled strategies would be able to leverage upon the strengths of both top-down and bottom-up approaches. Achieving this aim would involve the development of a methodology that establishes a suitable approach to self-assemble a strategy.

The sub-objectives to support the aim are as follows

- To study self-assembly conceptually
- To translate the studied phenomena into methods and algorithms to self-assemble strategies for use in supply chains

1.2 Organization of this Thesis

The thesis is organized as follows.

Chapter 2 briefly presents a conceptual review of Self-assembly. The field of Self-assembly is, although relatively immature, is very wide, and yet, unexplored for the purposes of Supply Chain Management. The chapter presents a look at the science of Self-assembly, its prominent features and characteristics, a discussion to distinguish between self-assembly and self-organization.

Chapter 3 examines the concept highlighted in Chapter 2 and then translates it into a simulation model. In this chapter, the mechanisms to induce self-assembly are examined and then isolated for translation into a methodology and algorithm for self-assembly.

Chapter 4 introduces how Self-assembly concepts can be adapted into an algorithm to generate a Supplier Selection Strategy. In this chapter, the methodology of selecting an appropriate self-assembly model, representation of a strategy, and application and benchmarking of the algorithm is detailed.

Chapter 5 then concludes the thesis.

Chapter 2

Conceptual Review of Self-assembly

2.1 Introduction to Self-assembly

The fascination behind self-assembly comes from the idea of ‘making things’. ‘Making things’ is one of the central activities of humans, and throughout our history, we have developed an extensive set of tools and techniques that allow us to manipulate matter at scales ranging from tenths of nanometres to thousands of kilometres (Boncheva & Whitesides, 2005). Most of these tools and techniques have been created from a ‘top-down’ approach, that is, we ‘make things’ based on a formulation of the overall problem⁵. Nature, however, takes a completely different approach, and it is possible to interpret most natural processes to be ‘bottom-up’ rather than ‘top-down’.

Take for an example, the ‘making’ of a snowflake. A snowflake begins when water vapour freezes onto an initial crystal. A six-sided shape emerges as new water molecules arrange themselves to reflect the internal order of the crystal’s water molecule. The intricate shape of each snowflake arm is also constructed using the same internal order, but varies based on the atmospheric temperature and humidity experienced by the snowflake as it falls to the ground (National Oceanic and Atmospheric Administration, 2013). This bottom-up approach to ‘making things’ is seen in many naturally occurring complex systems, such as viruses, proteins (Philp & Stoddart, 1996), crystal structures, and galaxies (Pelesko, 2007). The remarkable-ness of such activities are that they are done without external guidance; there is no entity that assembles the water molecules onto crystals that grows into snowflakes that are significantly larger. The ‘making’ process is intrinsic to the involved elements and the end-product is dependent upon the environmental conditions at which the processes takes place.

⁵ This can be interpreted to be the influence of the Newtonian paradigm on our modern thinking -- that the workings of nature are like an elaborate clockwork ruled by deterministic laws, and that problems can be ‘split up’, dealt with, and put back together again. See Prigogine & Stengers (1984).

Such bottom-up processes without external guidance are generally referred to as self-assembly – nature’s approach to dealing with complex systems. When self-assembly is studied as a science, it is studied as the science of putting things together and it is defined as the process which small components automatically assemble themselves into large, complex structures (Doty, 2012; Whitesides & Grzybowski, 2002)⁶⁷. Simpler components, which are generally considered to be autonomous, possess neither storage nor computational capabilities to follow a master assembly instruction set. They are only imbued with a limited repertoire of behaviours as they interact with their local environment and other components, and thus limited in their usefulness. Therefore, the significance of self-assembly is in its function as a distributed bottom-up process to create complex and more sophisticated structures from simpler⁸ components.

2.2 Prominent Features of Self-Assembled Structures

Much of what is known about self-assembly appears to come from the field of nanotechnology, although in recent years, there have been plentiful outputs from the related fields of chemistry, biology, robotics, and materials engineering (Boncheva & Whitesides, 2005; Doty, 2012; Groß & Dorigo, 2008; Lee, 2008; Pelesko, 2007; Philp & Stoddart, 1996; Whitesides & Boncheva, 2002; Whitesides & Grzybowski, 2002). To date, the prominent features of self-assembled structures have been recognised to be robustness, reversibility, and versatility⁹.

1. **Robustness** in many self-assembled structures comes in the form of redundancy, where the self-assembled structures is comprised of large numbers of components that can replace one another in the case of failure.

⁶ Other more specific definitions include: “the spontaneous generation of order in systems of components” (Boncheva & Whitesides, 2005); “the spontaneous formation of organized structures through a stochastic process that involves pre-existing components, is reversible, and can be controlled by proper design of the components, the environment, and the driving force” (Pelesko, 2007).

⁷ A write up on the history that led to the formation of the definition is presented in Pelesko (2007)

⁸ Simple as compared to the more complex aggregate.

⁹ Doubtlessly, there are many more features to be observed in self-assembly systems, an extensive elaboration could be done, but is not within the scope of this thesis.

Such structures have demonstrated robustness through their tolerance of errors and perturbations, and changes on its functionality to eventually recover by means of adaptation to the environmental changes (Groß, Bonani, Mondada, & Dorigo, 2006; Nagpal, 2002; Winfree & Bekbolatov, 2004).

2. **Reversibility** usually arises from adaptive cycles of association and dissociation in response to specific environmental cues. The advantages of such behaviours include the ability for components to readjust themselves to form aggregates without defects (Boncheva & Whitesides, 2005), and the ability to re-orienteer or steer the components into desired structures (Grinthal et al., 2012; Klajn, Bishop, & Grzybowski, 2007; Matsunaga, Aizenberg, & Aizenberg, 2011). Whereas in certain applications, stability is required, other applications might favour reversibility.
3. **Versatility** in self-assembly gives the possibilities for alternative, potentially superior, structures with new properties and/or applications. This is usually demonstrated through the ability for the components to re-configure the way in which they interact to each other though, for an example, electrostatic attraction and repulsion (Faul & Antonietti, 2003; Stang & Olenyuk, 1997).

2.3 Characteristics of Self-assembly

While there are many fields in which self-assembly has been explored, perhaps the most fertile field is in molecular self-assembly. Molecular self-assembly offers much insight and knowledge because of its ubiquity in chemistry, materials science, and biology (Whitesides & Boncheva, 2002), and that it has sufficient maturity to demonstrate the viability of self-assembly as a technique for manipulating matter and synthesis. In their work, Whitesides & Boncheva outline five characteristics of successful self-assembly in molecular systems (Whitesides & Boncheva, 2002). These five characteristics are: components, interactions, reversibility, environment, and mass transport and agitation.

1. **Components** are the basic molecules or segments of a macromolecule of a self-assembling system that interact with each other and are not necessarily required to be similar or different. The collective result behind their interactions with each other is a transition from a less ordered state (e.g. a solution, disordered aggregate, or random coil) to a more ordered final state (e.g. a crystal or folded macromolecule).
2. **Interactions** between components are the key activities within self-assembly. In molecular self-assembly, the interactions tend to be weak and non-covalent and their steady-state positions balance attractions and repulsions between components. For structures of meso- or macroscopic size, it is often possible to select and tailor the interactions between components to form desired structures.
3. **Reversibility (or Adjustability)**, mentioned in a prior section, is also identified as a characteristic that is important for self-assembly. If molecules are agitated and ‘stick’ together in an irreversible manner, glasses¹⁰ rather than crystals would be formed.
4. **Environment**. Molecular self-assembly usually occurs in solutions or in a medium that allows components to be mobile with respect to one another. Mobility allows the components to ‘move’ to balance attractions and repulsions and strongly influences the course of the self-assembly process.
5. **Mass Transport and Agitation**. Since interactions are critical for self-assembly to occur, the components must be mobile and induced into motion (or agitated). When in solution, thermal motion is often the common means used in molecular self-assembly to bring molecules into contact with each other. Assuring the mobility and choice of interactions between

¹⁰ Or, a frustrated system. Glasses are a type of frustrated system. A frustrated system can be understood as a complex system in which the components are stuck in non-trivial positions and have conflicting inter-component attraction/repulsion forces. See Chowdhury (1986).

components are therefore essential considerations to make in designing a self-assembling system.

2.4 Self-organization vs. Self-assembly

One ongoing debate in Self-assembly and the latest developments in Complexity Science has been the debate to distinguish between Self-organization and Self-assembly. This expected because in most research fields, there is no distinction between the two. A biologist, for example, would see no distinction between the two. Both Self-organization and Self-assembly are mechanisms for obtaining individual-based structures in which only the constituents take part ((Pitts, Graham, & Wareing, 1976; Sendova-Franks & Franks, 1999) as cited in (Halley & Winkler, 2008)) especially in bivouacs, bridges, and other complex collective structures in insect societies ((Anderson, 2002; Anderson, Theraulaz, & Deneubourg, 2002; Sendova-Franks & Franks, 1999) as cited in (Halley & Winkler, 2008)). In many observable phenomena, both Self-organization and Self-assembly can simultaneously occur (Halley & Winkler, 2008).

The most comprehensive effort so far, to distinguish between both concepts, can be found in Halley & Winkler's (2008) work¹¹. In Halley & Winkler's proposed distinction, Self-organization and Self-assembly can be distinguished in terms of equilibrium and thermodynamic arguments (Halley & Winkler, 2008). Self-organization can be interpreted to be a process that creates a dissipative non-equilibrium (or far-from-equilibrium) order at macroscopic levels from the collective, non-linear interactions between multiple components at the microscopic level. This order is induced by interplay between intrinsic and extrinsic factors, and decays upon the removal of the energy source. Self-assembly, on the other hand, is creates a non-dissipative structural order at the macroscopic level from the collective interactions of multiple components at the microscopic level that do not change their character upon integration into the self-assembled structure. Spontaneity in self-assembly occurs because the energy of unassembled

¹¹ See Bensaude-Vincent (2009) for an account of the more significant historical attempts at establishing the distinction.

components is higher than that of the self-assembled structure. As the components get agitated and self-assembles, an equilibrium is reached, and it persists without the need for energy input. To avoid a long exposition upon the intricacies of the differences between Self-organization and Self-assembly given Halley & Winkler's published effort, this thesis presents the summary of features and differences in Table 1¹².

While comprehensive, the definitions suggested by Halley & Winkler's work can be judged to be overly complicated. With the many criteria, it becomes cumbersome to classify observed phenomena, especially when the phenomena display different degrees of membership to each extreme. This is evident in their work through the cited examples of phenomena that exhibit both self-organization and self-assembly behaviours and mechanisms.

For a more inclusive distinction, the distinction proposed by Whitesides & Grzybowski is adopted instead. In their work, they suggest two main kinds of self-assembly: static and dynamic (Whitesides & Grzybowski, 2002). Static self-assembly denotes the process in which the ordered structure appears when the system reaches equilibrium, whereas in dynamic self-assembly, the ordered structure only occurs if the system is dissipating energy. The concept of self-organization, to Whitesides & Grzybowski, is described to be a form of dynamic self-assembly, and is evidenced in the examples that they cite in their work.

The rationale for adopting Whitesides & Grzybowski's distinction are: first, Whitesides & Grzybowski's stance stem from a long history of prior research, with Whitesides being a pioneer and major influence in the field of self-assembly; second, the distinction opens a wide range of potential exploration efforts, thus not forcing one to dichotomously choose between focusing on either concept; third, their suggested distinction is sufficiently simple and clear cut enough for comprehension.

¹² Other perspectives that were examined, but not included in Table 1 come from Anderson (2002), Svenson (2004), and Sendova-Franks & Franks (1999). These perspectives were excluded mainly because their definitions were not sufficiently flexible to be applicable in a cross/multi-disciplinary manner.

Feature	Self-organization	Self-assembly
Type of interactions	With the local environment throughout positive/negative feedback and with other components	With the local environment throughout positive feedback and with other components
Type of systems	Operative in open systems, i.e. require inputs/outputs of energy and matter	Restricted to closed systems, i.e. absence of inputs/outputs of energy or matter
Type of components	Autonomous components with general rules of interaction	Autonomous components with specific rules of interaction
Type of structures	Structures tend to be more general and variable, Stability of the structures are accompanied by energy dissipation and gain and loss of material	Well-defined, uniquely determined by the size, number of components, geometry, and strength of interactions amongst components
Thermodynamic state	Structures emerges from far-from-equilibrium processes involving energy/matter flow	Structures emerge by means of close-to-equilibrium dissipative processes which minimise the energy of the system
Requirement for initial coding	Does not require initial encoding and differences among components are not required	Global order of the assembled whole is dependent on the initial difference and/or specific relationships amongst components
Minimum number of components required	In many systems, a minimum threshold exists	Most self-assembled systems do not appear to have a minimum size requirement

Table 1: Features and differences between self-organization and self-assembly.
Adapted from Terrazas (2008), with additions from Halley & Winkler (2008) and Martin et al. (2008)

2.5 Onwards to Self-assembly

With concepts and distinctions made, it is now possible to proceed with inducing self-assembly.

Chapter 3

Self-assembly of Power Structures in Supply Chains¹³

The focus so far has been self-assembly in natural systems, but the study of self-assembly is not limited to natural systems. Self-assembly has also been studied in engineered systems¹⁴ as an engineering methodology. Like natural systems, the final self-assembled structure is encoded both in the interactions of amongst components and with the environment. Typically, this is done by embedding a careful design into the components (e.g. a shape or specific binding sites) or by specifying rules that the components follow. Carefully designed components typically take on an approach that focuses on fixed interaction rules and flexible goals, whereas the approach of specifying rules typically involve assigning different rules on components to achieve a fixed goal. Significant efforts of such an approach include Wang Tiles (Wang, 1961), Origami Shape Language (Nagpal, 2002; Nagpal, Kondacs, & Chang, 2003), and the Tile Assembly Model (Winfree, 1998). Such efforts can be considered a form of Templated Self-assembly¹⁵.

One requirement for Templated Self-assembly is for the self-assembly instructions to be encoded within the components and environment to ensure the emergence of a desired structure. Variations and deviations in Templated Self-assembly are thus an undesirable effect. This is, however, very different from its other variant – Biological Self-assembly. The prominent characteristic of Biological Self-assembly is the variety and complexity of the functions that can be produced (Whitesides & Grzybowski, 2002). This variety and complexity is made possible because in Biological Self-assembly, especially in living cells, total control of the parameters that determine the behaviour of the environment, components, and interactions between them is a luxury that is difficult, if not impossible,

¹³ The work in this chapter has been published in Yee, Ong & Tan (2015).

¹⁴ Or man-made systems

¹⁵ From Whitesides & Grzybowski (2002), “*In templated self-assembly, interactions between the components and regular features in their environment determine the structures that form*”.

to achieve. Such a setting is highly relevant to supply chains, because, like biological systems, each entity behaves individualistically and possess different motivations that are difficult, if not impossible, to completely control.

3.1 Self-assembling a Reproducible Pattern

As a development towards a Self-assembly methodology for supply chains, an attempt was made to mimic self-assembly behaviours in a supply chain. This is accomplished in the work of Yee, Ong & Tan (2015), where it was demonstrated that order, in the form of the supply chain taking on a certain power structure, can be induced from disorganized components at the micro level¹⁶. In the context of Complexity Theory, which the work was written for, the order that emerged was a result of self-organization, or dynamic self-assembly as recognised by Whitesides & Grzybowski (Whitesides & Grzybowski, 2002). Real-life supply chains, widely recognised as Complex Adaptive Systems (Choi et al., 2001; Pathak et al., 2007; Surana et al., 2005), have the inherent capability to cope with changing environments while seeking equilibrium. This ‘coping’ is reflected in the changes within the decisions made by firms to further their interests. Since no single firm pulls all the strings in the supply chain, the entire environment which the supply chain belongs to changes on its own to organize itself into a state of equilibrium or order. The objective of the work was to investigate the possibility of inducing a specific structure by imbuing the components (or firms) with the appropriate adaptive mechanisms that are like adaptive mechanisms seen in biological self-assembly. In the context of Self-assembly, this can be interpreted as a demonstration of ‘forcing’ a dynamic system into a reproducible pattern by encoding the relevant self-assembly instructions.

3.2 Simulation Model

The model was created using NetLogo (Wilensky, 1999) as a generic model of a three-tier supply chain, in which firms would trade and jostle for advantage

¹⁶ Yee, Ong & Tan (2015) used *agents* as it was created as an agent-based model, here *components* is used instead to retain consistency.

against each other. For simplicity, the traded goods in the supply chain were modelled to be homogeneous and non-perishable, and all firms act as price takers. The supply chain was modelled as an agent-based simulation model where firms were represented as individual components and the market environment as the system to make it analogous to the component-system configuration of typical self-assembly systems. The interactions between the firms gave rise to the variety of possible supply chain configurations¹⁷. These interactions, more descriptively, occurred between firms that are placed in a market environment in which they are free to discover and interact with each other. Whilst the firms can be aware of each other, they are not obligated to take actions that preserve or maintain the relationship formed between. And, at each time an interaction occurs, firms evaluate their available partners, and prioritise the ones that considered attractive¹⁸. However, the way the interactions occur are not static. Firms are imbued with simple adaptive mechanisms that allow them to adjust their internal parameters and evolve, thus modifying their attractiveness to other firms.

The concept of ‘energy’ in Whitesides & Grzybowski (Whitesides & Grzybowski, 2002) is represented by the flow of goods within the model. Goods enter and leave the environment by means of specific agents that introduce and remove goods from the supply chain. ‘Energy’ is dissipated¹⁹ when the goods are transformed into other goods by firms after purchase. Firms are also mobile in the sense that they are free to choose between different partners and are ‘agitated’ into action when there is demand for its goods.

3.3 Results

To track the change in power structure, the most appropriate measure was found to be the Herfindahl-Hirschman Index (HHI) (Hirschman, 1964; Rhoades, 1993; U.S. Department of Justice & Federal Trade Commission, 2010). The HHI is an economic concept that takes into account the size distribution of firms within a

¹⁷ Configuration as in the arrangement of components that give the whole its form. In Yee, Ong & Tan (2015), the focus was on the power structure, or influence relationships, between firms where its’ influence relates to the market share and power that it would hold.

¹⁸ In Yee, Ong & Tan (2015), the firms interact whenever they engage in trading activities with each other.

¹⁹ Dissipation can be understood to be a process in which energy is transformed from some initial form to another form.

market, taking value close of zero when the market is occupied by large numbers of firms with relatively equal power and rising to a maximum of 10,000 when a single firm controls the market. The power (or market share) of a firm was dictated to be the ratio of the quantity of goods demanded of it over the total quantity of similar goods demanded by all firms in the model within a time period.

In conducting the simulation runs, the values of a set of four parameters²⁰ were varied and left to run in the simulation model for 500 time-steps or periods. It was demonstrated that, by adjusting the initial parameters of the components and the system, it was possible to induce, with some reproducibility, a desired power structure or pattern (see Figure 1, Figure 2, Figure 3, Figure 4, and Figure 5 for results).

Figure 1. The effect of varying values of ρ on the HHI for each tier. For all cases, the following parameters are applied to all nodes: $\alpha = 5$, $\Delta p = 1$, and $\Delta c = 125$. Two lines are also included as visual indicators when the HHI is greater than 1500 and 2500. In (a) & (d), $\rho = 0.1$; in (b) & (e), $\rho = 1.0$. (c) & (f), presents the results where nodes have perfect discovery of their upstream suppliers, i.e. all upstream suppliers are revealed. This extreme case was investigated because values of $\rho > 1.0$ produced results that were uncannily similar. From these results, it can be observed that with increasing values of ρ , the length of time needed for the structure of high-power concentration to emerge is shorter²¹. From Yee, Ong & Tan (2015)

²⁰ The four parameters are: (1) ρ , the probability to discover new upstream suppliers; (2) Δc , handling capacity growth increment; (3) Δp , the price growth increment; and (4) α , the rigidity threshold.

²¹ This can be interpreted by observing the HHI values for each graph. Whenever the value of HHI exceeds 1500 or 2500, a structure of moderate or high concentration was reached.

Figure 2. The effect of varying values of Δc on the HHI for each tier. For all cases, all nodes have perfect visibility of their upstream supplier nodes and the following parameters $\alpha = 5$ and $\Delta p = 1$ are applied. In (a) & (d), $\Delta c = 5$; in (b) & (e), $\Delta c = 25$; and in (c) & (f), $\Delta c = 125$. From these results, it can be observed that with increasing values of Δc , the length of time needed for the structure of high-power concentration to emerge is shorter. From Yee, Ong & Tan (2015)

Figure 3. The effect of varying values of Δp on the HHI for each tier. For all cases, all nodes have perfect visibility of their upstream supplier nodes and the following parameters $\alpha = 5$ and $\Delta c = 125$ are applied. In (a) & (d), $\Delta p = 1$; in (b) & (e), $\Delta p = 5$; and, in (c) & (f), $\Delta p = 25$. From these results, it can be observed that with increasing values of Δp , the length of time needed for the structure of high-power concentration to emerge is shorter. From Yee, Ong & Tan (2015)

Figure 4. The effect of varying values of α on the HHI for each tier. For all cases, all nodes have perfect visibility of their upstream supplier nodes and the following parameters $\Delta p = 1$ and $\Delta c = 100$ are applied. Unlike the other experimental runs, a lower value Δc is applied to 'slow down' the process of evolution towards a structure of high-power concentration power. In (a) & (d), $\alpha = 0$; in (b) & (e), $\alpha = 5$; and, in (c) & (f), $\alpha = 10$. From Yee, Ong & Tan (2015)

Figure 5. Continuation of the results presented in Figure 4. In (a) & (d), $\alpha = 15$; in (b) & (e), $\alpha = 20$; and, in (c) & (f), $\alpha = 25$. From these results, it can be observed more obviously that with increasing values of α , the length of time needed for the structure of high power concentration to emerge is shorter. From Yee, Ong & Tan (2015)

3.4 Summary

The effort in Yee, Ong & Tan (2015) represented a first attempt at making use of known knowledge in Templated and Biological Self-assembly to create a form of reproducible order in a supply chain simulation. The results are conclusive that it is possible to apply Self-assembly principles in Supply Chains Management to achieve a certain level of predictability and order, albeit on a simple simulation model.

Chapter 4

Towards an Algorithm to Self-assemble Strategies²²

Whereas the work of self-assembling a structure for supply chains is interesting, it can be argued that it presents little value to practitioners aside from being an academic curiosity that highlights the complex nature of a supply chain. Practitioners in Supply Chain Management care for operational techniques that lead to real-life value-creation or cost-reduction activities, and Self-assembly provides a novel opportunity for that – the self-assembly of solutions to a problem. For example, the self-assembly of strategies that lead to better performance for a supply chain process.

The difficulty of developing this capability, however, is in the manner of which Self-assembly has been studied thus far. The great body of literature currently focuses on self-assembly techniques that manipulate matter, itself a non-trivial task and an immature field. Self-assembling a strategy would, therefore, require that existing concepts be translated and re-interpreted such that it would be suitable for use in engineered systems and field that it is to be applied to.

In the following sections, the work published in Yee, Ong and Tan (2016) are presented to detail the creation of a self-assembly algorithm and its application towards creating a supplier selection strategy.

4.1 The Many Self-assembly Systems

While mimicking a self-assembly system, a study was conducted to identify prior works on artificial systems that mimic assembly processes and assembled systems in self-assembly. From the results of the study, two distinct approaches were found: classical/mathematical models and simulation models. The significant

²² The work in this chapter has been published in Yee, Ong and Tan (2016).

works that were classified as classical/mathematical models include thermodynamic models²³, colloidal models²⁴, geometrical models²⁵, elastic models, and isotherms²⁶ (Lee, 2008). These works clarified self-assembly, but, because the focus of this effort is in the development of an algorithm, they were less impactful as compared to works involving simulation models.

Simulation models are relevant as they: (1) reveal both static and dynamic events of assembly (such as the kinetic pathway of assembly, disassembly, and reassembly); (2) permit the analysis of parameters that control the assembly process; (3) provide a understanding of the relationship between the structure of the assembled system and their properties and functions; and (4) provide a means to understanding the experimental results such that new assembled systems can be designed (Lee, 2008). In Lee (2008), simulation works were put into three major categories – electronic simulations (density function theory, mean field theory), atomistic simulations, and coarse-grained simulations. Of the many reviewed models, the Patchy Particle Model was found to be most relevant to this effort.

4.2 Patchy Particles

Patchy particles can be understood to be a class of particles that possess at least one well-defined discrete, attractive interaction site - a “patch” - through which it can experience an interaction with other particles or surfaces (Zhang & Glotzer, 2004). As an approach to fabricating complex structures, such particles function when they are conferred upon specific “instructions” on “patches” across their surfaces. As these “patterned” particles interact via strongly anisotropic interactions with other attractive “patches”, an ordered structure can be assembled from otherwise neutral or repulsive particles. Because the myriad of available variations that can occur due to size, shape and chemical, for the sake of brevity, an in-depth review into the state-of-the-art knowledge of the field patchy particles is avoided and the interested reader is referred to the work of Pawar and Kretzschmar (2010) and Bianchi, Blaak & Likos (2011).

²³ See Section 3.3 of Lee (2008)

²⁴ See Section 2.2 of Lee (2008)

²⁵ See Section 3.4 of Lee (2008)

²⁶ See Section 6.3 of Lee (2008)

4.3 Representing a Strategy

The starting point in devising a means to self-assemble a strategy is in devising a means to represent a strategy. In the context of Supply Chain Management, Operations Research or, generally, Business, a strategy is interpreted as a plan of action to designed to achieve a set of goals or objectives. To a computer, the same notion can be interpreted to be a series or sequence of actions that lead to a desired goal, which can be syntactically represented as a program tree with a specifically instructed tree structure. Therefore, in the interpretation of the self-assembly of patchy particles for strategy self-assembly, it is possible to interpret it to be similar to the creation of a tree where nodes are the equivalent of individual patchy particles and the number of available branches is analogous to the number of “patches” on each patchy particle (see Figure 6). These trees would self-assemble from singular nodes into more complex structures through various operators that take inspiration from the interactions in self-assembly systems. The patchy particles, or nodes for the purposes of a strategy tree, are represented by symbols of a function set $\{+, -, \times, \div, \dots\}$ and symbols of a terminal set $\{a, b, c, \dots\}$. The definition of these symbols in the function and terminal sets are inspired by the decision-making discipline. Elements from the function set represent the possible mathematical relationships between the different symbols of the terminal set, which are interpreted as pieces of information that are used and contribute to the decision outcome.

Figure 6. Graphical expression of patchy particles taken from Li, Zhu, Lu & Sun (2016). (a) Two patches regularly arranged in a linear geometry; (b) Typical patchy particle models with 1-4 patches, regularly arranged in spherical, linear, triangular, and tetrahedral geometries. By interpreting nodes of a tree as a patchy particle, we can mimic self-assembly interactions in our algorithm to create more complex structures.

To illustrate this, consider a simplistic low-cost strategy where the objective is to select suppliers based on their ability to offer the lowest total cost for shipping a quantity of goods. The symbols, or pieces of information, for this strategy would be the price for the quantity of goods P_{sell} , and the shipping price P_{ship} . The function set, or possible mathematical relationships between these two symbols would be $\{+, -, \times, \div\}$, where $\div$ would represent safe or protected division. Although all manners of relationships are possible, the most logical solution would be a strategy that determines the performance of the different suppliers by adding the values of P_{sell} , and P_{ship} together. Thus forming a strategy that could be mathematically represented as $P_{sell} + P_{ship}$, or in prefix/Polish notation²⁷, as $+ P_{sell} P_{ship}$ (see Figure 7).

Figure 7. Expression Tree for a hypothetical Vendor Selection Strategy

²⁷ A common notation used to represent trees

4.4 The Self-assembly Algorithm Procedure

The general concept of the Self-assembly algorithm is the application of manipulation techniques that synthesizes specifically designed building blocks into structures without external interference. Such bottom-up approaches have advantages over top-down approaches. From the perspective of Supply Chain Management, bottom-up approaches utilize past experience to gain knowledge and understanding of the key issues and underlying reasons for a problem to develop solutions, as opposed to top-down approaches that develop solutions based on defined principles (Kotzab et al., 2006). As a science that is known to bridge both approaches (Whitesides et al., 2005), self-assembly is a viable alternative approach to generating good solutions. In the context of developing strategies, to self-assemble a strategy is to synthesize, from the bottom-up, components that organize themselves into feasible configurations guided by principles fabricated from the top-down.

The procedure of the self-assembly algorithm is designed to mimic the behaviour of a generic self-assembly system of molecular components and assemblies that is self-assembling towards a specific objective structure. For simplicity's sake, it is assumed that the objective structure is feasible, and that the entire system would either self-assemble towards the objective structure or a structure that is as close to or like it as possible. Within this generic system, components function as the basic building blocks upon which more complex assemblies are self-assembled from. The structure of the assemblies that are formed can be understood to be reliant on the number of 'patches' that are available on the individual components. These patches represent the collection of binding sites that the components possess and their propensity for binding with any other binding site of another component. When the system is agitated, the components and assemblies would interact with each other, causing binding interactions to occur. Supposing that the binding pair of components and assemblies form a stable connection, a new assembly would be created and be added to the system of components and assemblies. From a computational perspective, specific to this study, components with patches can be interpreted to be nodes of an expression tree; binding sites can be interpreted to be branches; binding interactions to be actions

that join or split trees; and an assembly would be an expression tree. These objects are illustrated in Figure 8.

Figure 8. Illustration of the components and assemblies in a self-assembly system. (a) A component unit with two binding sites; (b) an assembly consisting of two components engaging in binding interactions with each other; (c) a system consisting of a sample of possible components and sub-assemblies

Figure 9 provides an overview of the strategy self-assembly algorithm. Performing strategy self-assembly requires a preparatory task of identifying all the possible pieces of information regarding the environment in which the strategies are to be assembled for and organizing them into a terminal set of values that the algorithm can use. From there, the strategy self-assembly process would begin by initializing a collection of syntactically valid trees that might represent a strategy. This is accomplished by randomly choosing symbols from the terminal set and having them ‘interact’ with each other. Upon ‘interaction’, symbols from the terminal set would take a symbol from the function set and together form a new assembly. This new assembly can exist by itself or be treated as a sub-assembly that could combine with other symbols or sub-assemblies to form a more complex assembly. For this step, it is possible to take inspiration from the initialization methods that are common in evolutionary computing and form the collection of strategies using the *Grow* method. This method was chosen because it has a close resemblance to the natural self-assembly processes of ‘growing’ complex structures from singular components through random interactions with other components in a system. From a practical standpoint, it also inhibits the random formation of large trees that would significantly increase computational cost.

Figure 9. Procedure of the self-assembly algorithm used in in Yee, Ong and Tan (2016)

Unfortunately, it is quite unlikely that a good strategy could be randomly assembled and there is the need to repeatedly manipulate the existing strategies to self-assemble better ones. For this step, we take inspiration from reproduction methods in evolutionary computing and manipulate each tree using the *Displacement*²⁸ and *Substitution*²⁹ operations to form a new collection of assembled strategies. In *Displacement* operations, two strategy trees are chosen and then a sub-tree randomly selected from each. Next, the two sub-trees are exchanged resulting in two new trees that are different from the original sub-trees. In *Substitution* operations, a strategy tree is chosen, and a randomly selected node is replaced with a new randomly created node. Both these operators allow the creation of new strategies that did not exist before in the collection of assembled strategies.

Specific for molecular self-assembly methods, there are two additional manipulation techniques – *Addition* and *Elimination*. In *Addition* operations, a randomly selected terminal node is replaced by sub-tree node that is formed by a combination of the original terminal node with a randomly chosen terminal node and random function. Effectively, this lengthens the strategy tree just slightly enough so that it grows at a gradual rate. For *Elimination* operations, random sub-

²⁸ Equivalent operation in evolutionary algorithms is a single point crossover

²⁹ Equivalent operation in evolutionary algorithms is point mutation

trees are selected and one of the branches are replaced with a randomly selected terminal node, effectively shortening the strategy tree. The combined effect of the *Addition* and *Elimination* is designed so that diversity can be regularly injected into the population of strategies in gradual manner.

Figure 10. Simplified illustrations of self-assembly operations used. In this work, strategy tree depth starts at 5 and can grow up to 20.

Formally, we can consider an assembled strategy to be ‘good’ when its performance achieves a certain threshold that was set out for it. This can be done through the creation of an appropriate simulation model that is able to capture, make use of the strategy, and then determine the performance of the strategy

against several objectives. Supposing that a ‘good enough’ assembled strategy is found after this step, it is logical to halt the algorithm. Often, however, this is not the case and the algorithm would have to assemble better strategies for several iterations before a ‘good enough’ strategy will emerge. To avoid excessive computation, we added a step that makes use of a selection method to reduce the number of the assembled strategies to manipulate and evaluate between iterations. This step would correspond to the behaviour of selecting the most stable assemblies amongst all available assemblies for continued self-assembly.

4.5 Self-assembly of Supplier Selection Strategies

4.5.1 The Supplier Selection Problem

The choice of suppliers is important to a firm as the firm’s success is dependent on whom it decides to procure its material from³⁰. For a firm, the choice of ‘best value’ is more complicated than scanning pricelists and selecting the supplier with the lowest price. Good suppliers are those that offer products, services or have qualities that match or exceed the needs of the firm. To procurement staff, having a firm-wide strategy enables operational decision making with regards to supplier selection in the manner that is consistent with the business objectives of the firm. These daily decisions impact a firm’s bottom line and significantly affects the firm’s performance.

Designing and forming such strategies is a difficult task because of the complex and adaptive nature of the modern-day environment (Choi et al., 2001; Pathak et al., 2007; Surana et al., 2005). To illustrate this difficulty, Dickson’s work in 1966 had already identified 23 criteria that were relevant to supplier selection (Dickson, 1996). In more recent studies, it was found that the difficulty is not only complicated with more criteria for consideration, but also that the relevant set of criteria changes across firms with different objectives and industries (Easton & Moodie, 1999; Ellram, 1990; Kingsman, Hendry, Mercer, & Souza, 1996; Mummаланeni, Dubas, & Chao, 1996; Stamm & Golhar, 1993; Weber,

³⁰ A recent census found that materials consumption is the top business cost item and accounts for almost half of the total business costs for the manufacturing sector in Singapore (Singapore Economic Development Board, 2014).

Current, & Benton, 1991). The modern firm, therefore, has a non-trivial task in dealing with uncertainty and the pace of change, and finding balance between the increased, and often conflicting demands, from customers, markets and suppliers while trying to make sense of the complex world around them.

4.5.2 The Usefulness of Self-assembly

With such a long history and significance to profitability, the supplier selection problem has garnered a lot of research interest (Chai, Liu, & Ngai, 2013; De Boer, Labro, & Morlacchi, 2001; Degraeve, Labro, & Roodhooft, 2000; Ho, Xu, & Dey, 2010). In examining the papers covered in Ho, Xu & Dey (Ho et al., 2010) and Chai, Liu & Ngai (Chai et al., 2013), the vastly popular approaches are observed to be mathematical- and consensus-based techniques with a mixture of both top-down (i.e. principle-driven) and bottom-up (i.e. experience- or data-driven) approaches. Such approaches share a common shortcoming in their reliance on human attention and involvement when designing and forming strategies that guide operational decisions. For example, the results from data envelopment analysis (the most popular approach identified by Ho, Xu & Dey (2010)) are known to be highly sensitive to the choice of inputs and outputs, and having the participation of experts with domain knowledge and experience about supplier selection is critical, and; in mathematical programming approaches (the second most popular approach), significant amounts of time and attention are required by trained experts to formulate suitable mathematical models. Such dependencies on human attention and involvement are not unique to mathematical- and consensus-based approaches, they are also relevant to the artificial intelligence and machine learning approaches identified by Ho, Xu & Dey (2010) and Chai, Liu & Ngai (2013).

In the modern world where change is ever occurring, the natural consequence of such approaches would be an increasing amount of time, money, and commitment required by firms to form good strategies. This is often motivated by the perceived need to achieve capabilities of prediction and control over its environment. However, it is found that such attempts often lead to frustration and helplessness as managers struggle with the dynamic and complex nature of their supply networks and the inevitable lack of prediction and control (Choi et al., 2001).

As an autonomous means to synthesize strategies that can be used supplier selection, self-assembly is significant as it reduces the amount of human attention and involvement to develop strategies that can be applied to real-world problems.

4.5.3 The Simulation Model

To showcase the ability of the algorithm to assemble logical strategies, a generic agent-based simulation model of a 2-tier supply chain with multiple suppliers and a single buyer was implemented. The numerical values used in the simulation model to represent the profiles of the suppliers $S_1, \dots, S_{10}$ to buyer B are presented in Table 2. The data for each supplier (in Table 3) is synthetic and was crafted to create three general types of suppliers (low-end, mid-range, and high-end) with sufficient variation such that the effectiveness of the self-assembled strategies can be obviously observed³¹. In testing out each strategy, the simulation model was created with the following assumptions:

- There are no limiting resources other than the amount of stock held by the suppliers
- There are no interruptions in the supply chain
- Orders are independent of each other, and order sizes are dynamic
- Any detected defects would be replaced by the supplier at no monetary cost to the buyer; and the buyer is assumed to ship goods that are defect free
- The price of products will not depend on the order lot size (no discounted prices)
- Suppliers will have processing capacity constraints, but no storage constraints; the total generated demand of the market will not exceed the total processing capacity of the suppliers

³¹ Many attempts were made to gather and use real-world data. Unfortunately, the real-world data was not possible to achieve sufficient variation such that the suppliers could be distinctively separated to give sufficiently meaningful results. There is a logical explanation for this phenomena - the market environment in Singapore is very competitive (price-wise) and the motivation to be price competitive is reinforced by a prevalent business practice of getting multiple quotes and going for the quote with the lowest cost. Thus, in many cases, suppliers tend to differentiate themselves by their after-sales services. Unfortunately, the dynamics of after-sales service is difficult to model and would unnecessarily complicate the simulation model. Since the purpose of the paper is to demonstrate the feasibility of self-assembling a strategy, it was therefore decided to use synthetic data and, perhaps, explore the use of real-world data in future works.

- The lead time between suppliers and the buyer is deterministic, and the demand for goods to the buyer would be stochastic

<i>Agents</i>	S_1	S_2	S_3	S_4	S_5	S_6	S_7	S_8	S_9	S_{10}
Selling price per unit	7	8	9	14	15	15	16	25	26	27
Fixed shipping cost per order	190	200	210	290	300	310	320	490	500	510
Shipping cost per unit	10	11	12	20	21	22	23	30	31	32
Processing capacity	1900	1600	1500	1600	1700	1400	1500	1500	1600	1900
Quality rejection rate (%)	6.1	5.7	6.2	3.1	3.2	3.5	3.4	1.2	0.9	1.1
Lead Time (days)	11	12	14	5	8	6	7	1	3	2

μ, σ of system demand 5000/250

Table 2. Numerical values of the simulation model used in Yee, Ong and Tan (2016)

Symbol	Description
\$0	Supplier's selling price
\$1	Supplier's fixed shipping cost
\$2	Supplier's shipping cost per unit
\$3	Supplier's processing capacity
\$4	Supplier's available stock
\$5	Supplier's quality
\$6	Supplier's lead time
\$7 - \$16	Numerical constants from 0 to 9
Function set	+, −, ×, and protected division %

Table 3. Terminal and function sets used in Yee, Ong and Tan (2016)

Although the algorithm is designed to generate strategies that can satisfy multiple objectives, the investigation limits itself to single objective applications as the focus is on operational level decision making. The objectives that were used to guide the self-assembly procedure are: (1) to minimize the total purchasing expenses made by the buyer agent; (2) to minimize the number of incoming defects by the buyer agent, and; (3) to minimize tardiness or the number of late deliveries by the buyer agent. These objectives were selected as they are the most

used operational objectives for the supplier selection. The parameters used in the self-assembly algorithm are presented in Table 4.

Parameter	Value
# of strategies	200
# of iterations	500
Mutation	Subtree mutation (5%)
Crossover	Subtree crossover (90%)
Maximum depth	8
# simulation runs	20 independent runs per strategy

Table 4. Parameter settings used in Yee, Ong and Tan (2016)

4.5.4 Results

The experiment results using the strategy self-assembly algorithm are documented in Table 5 and in Figure 11. Three independent experiments with different objectives were performed, and the best performing strategies for each experiment are indicated as *Strat1*, *Strat2*, and *Strat3*. These three strategies are self-assembled respectively to suit cost minimizing, quality maximizing, and tardiness (late deliveries) minimizing objectives.

In all three experiments, the selection decisions guided by the self-assembled strategies were compared against a random strategy (i.e. suppliers are selected randomly). As expected, in each experiment, the self-assembled strategies performed better than the random strategy and therefore demonstrates the viability and usefulness of the algorithm.

Strategies	Strat1	Strat2	Strat3
<i>Supplier Rank</i>			
S_1	2	5	10
S_2	5	7	7
S_3	8	9	5
S_4	10	8	2
S_5	3	10	8
S_6	9	4	1
S_7	7	6	4
S_8	6	1	3
S_9	4	3	6
S_{10}	1	2	9
<i>Performance</i>			
SA Strategy	\$11.91M	1.35%	17
Random Strategy	\$20.20M	3.33%	33

Table 5. Experiment results conducted in Yee, Ong and Tan (2016)

Figure 11. Performance of self-assembled vs. random strategies in Yee, Ong and Tan (2016)

4.6 Benchmarking the Self-assembly Algorithm

With the success of self-assembling strategies that can be used for the supplier selection problem, it becomes important to be able to compare the performance of the algorithm against others. A good candidate is the Genetic Programming algorithm by Koza (1994). As a population-based evolutionary computation algorithm, the Self-assembly algorithm shares many traits with Genetic Programming, such as the need to iterate between different populations of solutions, trimming the population to ensure efficiency, and the use of operators to manipulate the makeup of the population. Where Genetic Programming encodes programs

as a set of genes, Self-assembly encodes strategies as a set of decision variables. These traits make Genetic Programming algorithms a good comparison to benchmark the performance of the algorithm. A summary of the similarities and differences are highlighted in Table 6.

Feature	Self-assembly	Genetic Programming
Inspiration	Molecular self-assembly	Natural selection
Types of initialization	Grow	Grow, Full, Ramped-half-and-half
Types of operators	Addition	Crossover
	Substitution	Mutation
	Elimination	
	Displacement	

Table 6. Comparison between Self-assembly and Genetic Programming

To ensure fairness in the comparison, the Self-assembly algorithm was adapted for use in a symbolic regression solver³². Symbolic regression was chosen because it is a common task that Genetic Programming algorithms are regularly benchmarked against, and that there are many known functions in the literature that have been used to extensively study the various behaviours of both algorithms.

For the symbolic regression problems, five test problems were chosen. For reference, the problems featured in Kattan, Agapitos, Ong, Alghamedi, and O’Neill (2016) were used (See Table 7). The experimental settings, such as function and terminal sets, training data, parameters (See Table 8) were also retained. The computation results of the experiment are presented in Figure 12.

³² This was implemented as a straightforward application that was designed to find the best fit function for a set of paired data between a dependent variable Y and a given independent variable X . The objective was to benchmark the Self-assembly algorithm against Koza (1994)’s Genetic Programming algorithm.

Func- tions		Bound
F1	$f(x_1, x_2) = \frac{e^{-(x_1-1)^2}}{1.2 + (x_2 - 2.5)^2}$	[-2, 2]
F2	$f(x_1, x_2, x_3, x_4, x_5) = \frac{10}{5 + \sum_{i=1}^5 (x_i)^2}$	[-5,5]
F3	$f(x_1, x_2) = 6 \sin(x_1) \cos(x_2)$	[-5,5]
F4	$f(x_1, x_2, x_3, x_4, x_5) = x_1 x_2 x_3 x_4 x_5$	[-5,5]
F5	$f(x_1, x_2, x_3, x_4, x_5) = 32 - 3 \frac{\tan x_1 \tan x_3}{\tan x_2 \tan x_4}$	[-5,5]

Table 7. Test problems used in Kattan, Agapitos, Ong, Alghamedi, and O'Neill (2016)

Parameter	Value
Population size	200
# of iterations	500
Crossover / Displacement	70%
Mutation / Substitution	30%
Addition	30%
Elimination	30%
Maximum depth	10
# simulation runs	5 independent runs
Terminal set	Numerical constants from 0 to 9
Function set	+, -, ×, and protected division %

Table 8. Settings used in the benchmarking experiments

Figure 12. Performance of the Self-assembly algorithm vs. Genetic Programming algorithm

As presented in Figure 12, the average performance of the Self-assembly algorithm beats the performance of the Genetic Programming algorithm in 4 out of the 5 test problems. In these four test problems, it can also be noted that the

Self-assembly algorithm converges faster and achieves a better fitness value as compared to the Genetic Programming algorithms. These results have two interpretations: the first, the Self-assembly algorithm can be competitive with other evolutionary algorithms in the literature, and the second, the performance of the self-assembled strategies presented in Section 4.5.4 can be proven to be legitimately generated.

4.7 Summary

The Self-assembly algorithm successfully self-assembled strategies for the supplier selection problem for three different test cases derived from objectives used in the real world. The algorithm functioned, as it was designed, by focusing on exploring and discovering suitable structures and pieces of information that are needed to achieve the set of targeted objectives that were defined for the purpose of the supplier selection. With the simple requirements of only having to declare a set of objectives and provide pieces of information (whether relevant or not), the self-assembly algorithm was an approach that bridges between the traditional top-down approaches and more recent developments with bottom-up approaches towards supplier selection.

For decision makers, this work is a significant development because it indicates a potential to understand a complex environment without explicit domain knowledge nor a need to make assumptions on available information. This allows for faster speed and flexibility in developing strategies to accommodate the changes in the complex modern-day environment as they occur.

Chapter 5

Conclusion

This thesis may be divided into two parts. Chapter 2 presented a conceptual overview of self-assembly. Chapters 3 and 4 extended from the concepts presented in Chapter 2 and translated them into a simulation model and an algorithm that mimics self-assembly mechanisms. With the work presented in Chapter 4, the objective of exploring the feasibility of self-assembling strategies for use in supply chains is now achieved. This chapter thus serves as the closing discussion for the effort.

5.1 Future Work

A logical next step of development for the methodology in Chapter 4 would be to expose it to more sophisticated problems. Right now, the effort expended is one that is conventionally expected of any Operations Research effort -- focusing on single problems. That is, problems are considered in isolation and not with related problems³³. However, such efforts are not reflective of what the real-world community needs (Michalewicz, 2012). Most firms run complex operations and they need solutions for problems that involve multiple sub-problems that interact with each other. A means to develop strategies that treats problems holistically³⁴ is one that would be practical to the modern-day firm and would be a significant contribution to research (Bonyadi & Michalewicz, 2016; Bonyadi, Michalewicz, Neumann, & Wagner, 2016).

In recent years, some effort has been expended into studying interdependent real-world problems as multi-component problems. The defining characteristic of multi-component problems is that they are a combination of multiple sub-

³³ For example, a strategy to schedule production lines (e.g. maximize efficiency or minimize cost) should have a relationship with strategies that determine inventory costs, stock-safety levels, replenishment targets, transportation costs, etc.

³⁴ That is, to take all sub-problems into account rather than only focusing on individual sub-problems.

problems with intricate dependencies amongst the problems. One real-world example is the tank delivery problem (Stolk, Mann, Mohais, & Michalewicz, 2013) mentioned in Bonyadi, Michalewicz, Neumann & Wagner (2016). The tank delivery problem is a combination of tank selection, delivery routing, base selection, and bundling. The solution for delivery routing (best route to deliver tanks) is affected by the base selection (best choice to unbundle the tanks) as choosing different bases imposes different lengths of travels between the base and stations. Delivery routing is also affected by the tank selection (selecting the best tanks for delivery) as the selected subset of tanks determines the stations to visit. With this example, it is easy to appreciate the interdependencies between the sub-problems and that the feasibility or best achievable solution for any sub-problem or component is affected by the solution of the other components.

In Bonyadi, Michalewicz, Neumann & Wagner's (2016) work, it was suggested that there are two possible approaches to solving multi-component problems. The first is to nest the different solvers for the different sub-problems within each other (i.e. multi-level optimization), and the second, is to use multiple isolated populations of solutions (i.e. coevolution) as a mechanism to create isolated subpopulations of individuals in a common ecosystem. Both approaches are theoretically sound, and as of writing, there are several published works utilizes either approach. Unfortunately, there is little comment on the effectiveness of either approach beyond speculative potential opportunities or successes. This is justified because the focus on multi-component problems is new and the availability of published efforts would be scarce. With that in consideration, it is thus reasonable to accept that the full comprehension of the opportunities and appropriate approaches is not available and that it is possible that there exist alternative approaches that are more suitable to solving multi-component problems.

One possible alternative, and possible extension of this, is to take a multitasking approach. The approach of multitasking, using computers, is inspired by the human's cognitive ability to multitask. From a Computer Science perspective, this is mimicked by performing a number of tasks in parallel and purposefully leveraging upon the relevant information between the different tasks using a shared representation space (Ong & Gupta, 2016). Multitasking works because the increased generalization of specific characteristics in the multiple sub-problems facilitates the inductive transfer of potentially rich information between the

population of solutions. Therefore, making it simpler to solve sub-problems together rather than solving the sub-problems in isolation.

Considering the psychologists have conceded that bundling together related tasks could potentially improve productivity (Adler & Benbunan-Fich, 2012; Dzubak, 2008; Salvucci & Taatgen, 2008), it is not unreasonable to accept that exploiting the latent synergies between distinct (but possibly similar) problems could achieve enhanced productivity and superior quality solutions (Da et al., 2016) for multi-component problems. This makes exploring the feasibility of the integrating multitasking approach and self-assembly methodology a credible and worthwhile effort to solving multi-component problems.

5.2 Ending Statements

This thesis details a study of the mechanisms that govern the autonomous synthesis of large, complex structures from small, simple components. These mechanisms are interpreted and converted into procedures that are used in an algorithm to autonomously generate complex solutions to problems by utilizing basic and discrete pieces of known information about the problem. Such a capability is significant for the complex modern world as time and human attention to study problems are luxuries that are increasingly difficult to afford.

At the beginning of this thesis, the widely acknowledged complexity in the modern supply chain was highlighted as a growing problem for supply chain managers. And, it was mentioned that more could be done to appreciate and act upon the complexity of the modern-day supply chain. Part of that call to do more is now realised via the effort presented in this thesis. The objective of this study was to develop a methodology for the self-assembly of supply chain strategies for use in supply chains. And, from the content presented in Chapter 3, the objectives were met, and it is demonstrated that it is possible to self-assemble strategies to address and solve supply chain problems.

The attractiveness of developed methodology is not so much in the novelty of its creation, but rather in its ability to ‘bridge’ the goals of both top-down and bottom-up approaches to strategy development. The top-down approach, rep-

resented by defining the fitness function, is complemented by the bottom-up approach of synthesizing new strategies by naively combining different pieces of information together and then selecting the best ones through a series of systematic evaluations.

The significance of the developed methodology is that it is an approach to address one of the sources of frustration and helplessness that plague modern-day supply chain managers – dealing with the dynamic and complex nature of their supply networks and the inevitable lack of prediction and control (Choi et al., 2001). Because the methodology enables the exchange of human attention and involvement with the ever-decreasing cost of computational resources, such a capability is valuable.

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