ANALYSIS OF COUPLING PARAMETERS FOR GRAPH COLOURING IN COMPLEX ADAPTIVE AND DYNAMICAL SYSTEMS FRAMEWORK*

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Abstract. Network of oscillators are studied to understand if graph (vertex) colouring can be obtained upon synchronization when a strong negative coupling is applied between oscillators when there is an edge present in the network and a small positive coupling is applied between oscillators when there is no edge. We find that oscillators with simple equations such as Thomas' systems are best suited for such couplings. We further observe that introducing a degree of variance in coupling strength improves synchronization to a great extent in favour of returning optimal graph colouring in such networks. We further study the role of parameters (which are obtained as a result of varying coupling strength) on synchronization. The present article thus ends up proposing a polynomial time heuristic method to solve the graph colouring problem.

Key words. Vertex Colouring, Coupled Thomas' systems, Asymmetric Coupling

AMS subject classifications. 05C15, 37M05, 37N40, 65L06

1. Introduction.

A simple system of study may be distinguished from a complex system as the latter may showcase some kind of emergent phenomenon under some sort of observation or analysis. Network theory as an interdisciplinary field of research has been developing primarily over the last two decades to model pairwise interaction in complex systems [20, 27]. Networks in a general sense find their origin in mathematical structures called graphs which have been rigorously studied through the formal axioms, definitions and theorems paradigm and graph theory is rather a much older discipline, the origins of which can be traced back to Euler's solution of Königsberg bridge problem [3, 29]. Thus while graphs are mathematical objects, networks can be distinguished from graphs by thinking them as a methodological representation of real world complex systems based on empirical data or problem oriented parameters [20].

Complex adaptive systems as a term can be thought of as a generalized research area that provides a spectrum of systems based methods, formulations or techniques for query into traditional individual research fields or modern interdisciplinary research fronts. A complex system under study can be classified as a complex adaptive system (CAS) if it is guided by three basic principles which are, a) diversity among components of a system, b) interaction among individual components of the system under study and c) a regulatory process or rules of interaction or system dynamics either known or hidden that govern the interaction among components at different level of organization (in a sense that a two body interaction is fundamentally different from a three body interaction and so on). Thus, a wide array of systems ranging from an individual cell in the body to ecology and environment of planet Earth can be studied as a complex adaptive system [13, 17, 18]. It must be well noted that since the turn of this century, networks are widely used to model complex adaptive systems.

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The study of complex adaptive systems can be further refined to include the exact known dynamics of components involved in the system in the form of differential equations (ODE or PDE) or difference equations etc., with a clear advantage that by modelling the system in such a manner, the traditionally well established methods and theories of dynamical systems (bifurcation and chaos for example) may be used to describe, probe or study the system at hand [2, 4, 5, 19]. One must observe that while individual components are described by their known dynamics, the system still can be modelled as a network by knowing or guessing the way in which each of the components may mutually interact with each other. The resultant approach to model a complex adaptive system in such a way gives birth to the study of complex adaptive and dynamical systems (CADS) [11, 10]. We must emphasize here that networks may still be used to model pairwise interaction among components in complex adaptive dynamical systems. The applications of dynamical systems theory to study dynamics of networks is thus a deeply involving field where numerous applications such as opinion dynamics, dynamics on networks with varied topology etc. are studied [15, 22].

In the present work based on CADS framework, we discuss the famous graph colouring problem in complex adaptive dynamical systems framework. Given a graph G, the graph colouring problem(more precisely the vertex colouring problem) is to find a partition of the vertex set of the graph in such a way that no two adjacent vertices have the same colour and such a colouring of the vertex sets is called a valid graph colouring. Moreover at the same time, if the the number of sets in such a partition is minimum then such a graph colouring is optimal. The cardinality of such a partition for witch the number of colours are minimum is called the chromatic number. To find the chromatic number is NP-hard, while to find such a partition is NP-complete for a given graph [9, 23, 14, 25]. The central objective of the present study is to come up a heuristic method that presents a valid graph colouring, given a graph G. Furthermore, we wish to find conditions under which such a graph colouring may turn out to be optimal.

In order to address the graph colouring problem in CADS framework, we try to develop a network of coupled oscillators such that these oscillators have either a positive or a negative coupling depending on the adjacency of network (i.e. underlying graph) in question. The positive and negative coupling between oscillators can also be viewed as attraction-repulsion coupling forces. There is a manifold inspiration behind choosing an attraction-repulsion coupling pair as a fundamental quality of interaction between agents (in this case oscillators) to study graph colouring in CADS framework.

Attraction-repulsion couplings manifest themselves in numerous systems starting from fundamental forces such as gravitational, electromagnetic and strong and weak nuclear forces, such that it may be possible that two given bodies may have a strong repulsive electromagnetic interaction between them but a relatively much weaker gravitational pull is also present at the same time. Likewise, at the molecular level, various forces such as ionic, covalent interaction and van der Waals forces describe a spectrum of phenomenon and molecular interactions. At an ecological scale too, the interactions with respect to carbon exchange between species can be thought of as either repulsive (as is the case with predator-prey and host-parasite kind of interactions, where one of the species involved is actively avoiding such interaction) or attractive (for instance in seed-dispersion and plant-pollinator networks, where carbon exchange is desirable for both the agents involved). Thus, in the present work we want to get an insight into the role of attraction-repulsion coupling pair on the nature of computations, in particular, how such basic interactions may lead to solutions to hard problems in nature (such as graph colouring as discussed here) though even for a small number of agents involved. Thus we study graph colouring as obtained upon synchronization of coupled oscillators.

We further wish to find the range in which the ratios of amplitudes of coupling strength between given oscillators may lie so that the oscillators synchronize (and hence form a partition of underlying graph) in such a way that the resultant synchronization is optimal graph colouring. However, we would first like to present a comprehensive mathematical outlook of the terminologies and methods used in this work for better clarity in conception for the reader and the same is done in the following section.

2. Brief Terminologies and Method.

In this section, we present a brief outline of terminologies and methods used in this work. We try to formally define the terms as far as possible and deviate from formal paradigm when we are solely interested in the application front of the problem at hand.

2.1. Graph Colouring.

Let $G = \{V, E\}$ be a graph. A partition $P = \{P_1, P_2, \ldots, P_n\}$ of the vertex set V, is a finite collection of non-empty subsets of the vertex set V, such that $P_i \cap P_j = \emptyset$ for all $i, j \in 1, \ldots, n$ and $\cup_i P_i = P : 1 \leq i \leq n$. Thus a partition is collection of subsets of a set P such that mutual intersection of the subsets is empty but the union of all the non-empty subsets is equal to the set P.

Given a graph $G = \{V, E\}$, the vertex colouring problem is to find a partition P of the vertex set V such that any two adjacent vertices do not lie in the same partition. Moreover, the vertex colouring (hereto referred as graph colouring) is optimal if the cardinality i.e. number of sets in the partition P is minimum and the corresponding number is known as the chromatic number of the graph G, most commonly represented as χ_G. To find a method that deterministically finds the chromatic number χ_G of a graph G is $NP-hard$. Moreover, to find a method which rather finds a partition deterministically, which is optimal graph colouring, is an instance of a $NP-complete$ problem.

2.2. Graph Colouring in CADS Framework.

We first present the graph colouring problem in complex adaptive dynamical system in an preliminary form. To form a network of coupled oscillators, first consider an oscillator given by the following generalized equations

$$\begin{aligned} \dot{x} &= f_x(x, y, z) \\ \dot{y} &= f_y(x, y, z) \\ \dot{z} &= f_z(x, y, z). \end{aligned}$$

To study the graph colouring problem in the CADS framework, for a given graph G, we couple the given oscillators in such a way that an oscillator corresponds to a given vertex in the graph and is coupled by a constant $-\alpha, \alpha > 0$ when there is an edge between two vertices and the coupling constant is $\beta, 0 < \beta << \alpha$, when there is no edge between the two given vertices. Thus for a given graph G we form a network of coupled oscillators by coupling every i^{th} oscillator by J^{th} oscillator, $i \neq j$, the generalized equation form for which can be described as

$$\dot{u}_i(t) = f_{u_i}(x, y, z) + \sum_{j=1, j\neq i}^{N} K_{ij}\left(u_i(t) - u_j(t - \tau_{ij})\right) \tag{2.1}$$

where $u_i = x_i, y_i$ or z_i and $K_{ij} = -\alpha$ if $(A)_{ij} = 1$ and $K_{ij} = \beta$ if $(A)_{ij} = 0$. A is adjacency matrix of the graph G and N is the order of the graph. Here τ is constant representing the time delay in coupling and in the present study it is considered to be 0.

In the present work we wish to develop a heuristic method that finds optimal graph colouring for a given graph G. In order to develop such a heuristic method, it is assumed here that the set of vertices that synchronise with each other under the coupling described in Equation 2.1 can be thought of as a set of vertices with same colour. Thus we may find a partition of the vertex set such that each set in the partition is set of vertices that have synchronized with each other. It is for us to find conditions upon the coupling parameters such that such a partition turns out to be an optimal graph colouring.

Synchronization in complex network is an active area of research [1, 7, 16, 21]. Coupling equations with a form similar to one presented in Equation 2.1 has been discussed in the literature. However, in our case we wish to employ the Range-Kutta methods (more precisely the simple RK4) to find numerical solutions to the the given equation form. The advantage of using RK4 as choice of method to solve the given equation numerically is that it is a known $O(n)$ (where n is the number of iterations for which the method runs) time complexity method with a small $(O(h^5), h \approx 0)$ residual error term. Only a few studies are known to authors that have tried to study graph colouring from a synchronization in networks point of view [24]. However, a study which employs numerical methods such as RK4 to achieve synchronization with an aim to address graph colouring problem is rather unknown to the authors and thus adds to the novelty of this work.

3. Results and Discussion. In this section we describe the evolution of our approach to search for optimal graph colouring for given graphs, beginning with Equation 2.1 as a starting point. The copupling parameters intitially are chosen as $\alpha = 10$ and $\beta = 1$, and we wish to find oscillators which are best suited to return a valid graph colouring under the given coupling instance.

3.1. Choice of Oscillators. For a given graph G, we start with coupling Chua's oscillators [6] to form a network of coupled oscillators such that each vertex of the network represents an individual Chua's oscillator with identical parameters and every oscillator is coupled with every other oscillators with coupling parameters as described by Equation 2.1.

The Chua's oscillator in the equation form can be described as

$$\begin{aligned} \dot{x} &= a(y - \phi(x)) \\ \dot{y} &= x - y + z \\ \dot{z} &= -by \end{aligned} \tag{3.1}$$

where $a, b \in \mathbb{R}$ and $\phi(x)$ is a piece-wise linear function in x, defined as

$$\phi(x) := m_1 x + \frac{1}{2}(m_0 - m_1)(|x+1| - |x-1|).$$

The choice of constants a, b, m_0 and m_1 in our case are 15.6, 28, -1.143 and -0.714 respectively. We start by using the smallest connected graph on three vertices i.e. P_3, path on three vertices as an initial reference graph, shown here in Figure 1.

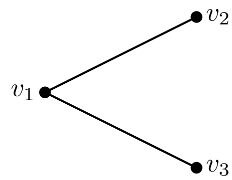

FIG. 1. *The path graph P_3*

For the graph P_3, given that i ranges from vertex v_1 to v_3, where v_1 is vertex with degree 2 and v_2 and v_3 are vertices with degree one, the coordinates x_i, y_i and z_i of a coupled Chua's oscillator i are presented in the plot shared as Figure 2.

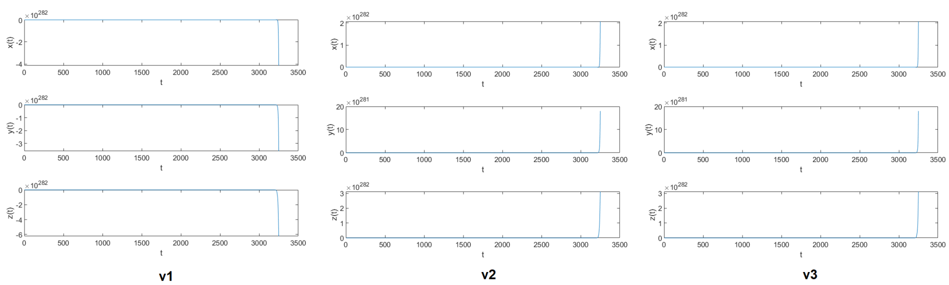

FIG. 2. *The change in coordinate values over time for coupled Chua's oscillators representing vertices v_1, v_2 and v_3, for the given graph P_3. The coordinate values change exponentially over time.*

It is observed that the coordinates for coupled oscillators representing vertices $v2$ and $v3$ overlap with each other and hence have synchronized. Thus $v2$ and $v3$ can be assigned the same colour, while oscillator corresponding to vertex $v1$, whose coordinates are different from vertices $v2$ and $v3$, is assigned a different colour, resulting in optimal graph colouring for the graph P_3. We also notice that as a result of choice of coupling equation the coordinates of the coupled oscillators are exponential in time. The overlap in the coordinate values for vertices $v2$ and $v3$ can be observed as Figure 3.

The aforementioned process is replicated for the remaining connected graph of order three, i.e. C_3 the three cycle and all connected graphs of order four with coupled Chua's oscillators as vertices and the results are summarized in Table 1. It must be notices that we have used the information system on graph classes and their inclusions (ISGCI) by H. N. de Riddler (https://www.graphclasses.org) as a standard nomenclature for most of the graphs mentioned in this work.

We further wish to access if choice of a different oscillator for coupling affects the synchronisation in different graphs. For the purpose we replace Chua's oscillator with a Rössler attractor [26], the equations for which are given below.

$$\begin{aligned} \dot{x} &= -y - z \\ \dot{y} &= x + ay \\ \dot{z} &= b + z(x - c), \end{aligned} \tag{3.2}$$

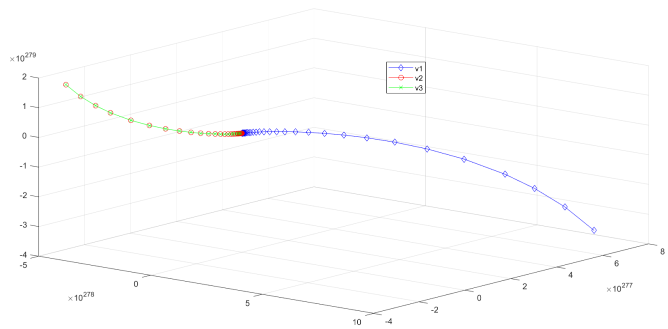

Fig. 3. *The change in coordinate values over time for coupled Chua's oscillators representing vertices v_1, v_2 and v_3, for the given graph P_3. The coordinates for vertices v_2 and v_3 are overlapping.*

where a, b and $c \in \mathbb{R}$ are parameter values chosen as 0.432, 2 and 4 respectively in our case. It is observed that for the choice of oscillator as Rössler attractor, coordinates for all vertices i in our initial reference graph P_3 are found to be different and there is no overlap between v_2 and v_3, thus returning a suboptimal graph colouring. Thus we conclude that a Rössler attractor is not a good choice of oscillator for our purpose. We furthermore conclude that in our scheme some oscillator are better than others in terms of producing synchronization that results in optimal graph colouring.

Thus we set out to find the best possible oscillator for coupling such that for such an oscillator optimal graph colouring upon synchronization is found for maximum possible graphs. We tried coupling oscillator systems such as Lorenz system [8] and Lotka-Volterra system (in two dimensions) [12] from a large number of known chaotic oscillator systems but could not improve on the results obtained for Chua's oscillator.

We find success in replicating the results obtained for Chua's oscillator by using Thomas' cyclically symmetric system [28]. The equations for Thomas' cyclically symmetric system are

$$\begin{aligned} \dot{x} &= sin(y) - bx \\ \dot{y} &= sin(z) - by \\ \dot{z} &= sin(x) - bz, \end{aligned} \tag{3.3}$$

such that the system becomes chaotic for choice of $b \approx 0.208106$. The results obtained for Thomas' system for the choice of b as 0.208106 are tabulated as Table 1.

It can be observed that the equations for Thomas' system are very simple. This leads us to try some other simple equations in lieu of Thomas' system. For instance, we remove the *sin* terms from the equations for Thomas' system to get the equations

$$\begin{aligned} \dot{x} &= -bx \\ \dot{y} &= -by \\ \dot{z} &= -bz, \end{aligned} \tag{3.4}$$

and we find that the results are still replicated i.e., the graphs that show optimal graph colouring upon coupling for Chua's oscillator and Thomas' system show optimal graph colouring for the changed equations. It is further observed that we find the same set of results getting replicated when we try other simple functions for coupling such as, $\dot{u} = c, c$ is constant, $\dot{u} = \frac{-cu}{(1+u^2)}$ for example, where u is x, y or z. This leads us to believe that the synchronization observed for different vertices that results in optimal graph colouring depends on the topology of the graphs in question. Thus choice of simple equations for coupling shall lead to maximum possible graphs returning optimal graph colouring, while oscillators with more complicated equations shall reduce this number.

3.2. Asymmetric Coupling. As we have noticed that the changes in coordinates over time for systems coupled in accordance with Equation 2.1 are exponential, we make a small initial change to the coupling equation so that the resultant change in coordinates is no longer exponential. The coupling equation is thus changed to

$$\dot{u}_i(t) = f_{u_i}(x, y, z) + \sum_{j=1, j\neq i}^{N} K_{ij} \frac{(u_i(t) - u_j(t))}{(1 + (u_i(t) - u_j(t))^2)} \tag{3.5}$$

where, as seen earlier, $u_i = x_i, y_i$ or z_i and $K_{ij} = -\alpha$ if $(A)_{ij} = 1$ and $K_{ij} = \beta$ if $(A)_{ij} = 0$ and for present $\alpha = 10$ and $\beta = 1$.

We tried to find graph colouring for all twenty one connected graphs of order five by coupling Thomas' system as per the equation given above. This gives us a system of $3N$ coupled equations derived from Equation 3.5, where N is the order of the graph. These equations for the coupled Thomas' system can be represented as

$$\dot{x}_i(t) = sin(y_i) - bx_i + \sum_{j=1, j\neq i}^{N} K_{ij} \frac{(x_i(t) - x_j(t))}{(1 + (x_i(t) - x_j(t))^2)}$$

$$\dot{y}_i(t) = sin(z_i) - by_i + \sum_{j=1, j\neq i}^{N} K_{ij} \frac{(y_i(t) - y_j(t))}{(1 + (y_i(t) - y_j(t))^2)}$$

$$\dot{z}_i(t) = sin(x_i) - bz_i + \sum_{j=1, j\neq i}^{N} K_{ij} \frac{(z_i(t) - z_j(t))}{(1 + (z_i(t) - z_j(t))^2)}, \tag{3.6}$$

where K_{ij} are coupling constants as explained earlier and b is a parameter for Thomas' system. We choose $b = 0.1$ for the rest of the study as a lower value of b helps reduce the sinusoidal fluctuations in the values of $\dot{u}_i$ over time.

We obtained numerical solutions of the above equations using the RK4 method and find that for connected graphs of order 5, only four graphs (which are $K_{1,4}, K_{2,3}, W_4$ and K_5) show an optimal graph colouring upon synchronization. The method returns a sub-optimal graph colouring for six graphs which are, $P_5, fork = chair, bull, P = 4 - pan = banner, C_5$ and $house = \overline{P_5}$, where $\overline{G}$ is the complement of a graph G. The remaining eleven graphs return an invalid graph colouring such that there is a pair of adjacent vertices in these graphs which are assigned the same colour upon synchronization.

On analysing the data i.e the coordinate values generated for different oscillators for a given graph, we conclude that apart from the topology of the graph there is a certain role played by symmetry in strength of coupling parameters that affects the synchronization leading up to optimal graph colouring. In principle, positive and negative coupling in oscillators can be thought of as attraction and repulsion forces that pulls the vertices of a graph (i.e. oscillators coordinates over time) towards each other or pushes them away from one another. Thus if due to the topology of the graph a situation arises where a vertex is free to synchronize with any k vertices with which it is not adjacent, it will not be able to synchronize with either one of the k vertices as it is pulled towards all the k vertices with equal coupling strength. The situation can be illustrated with the help of graph C_5, shown here as Figure 4.

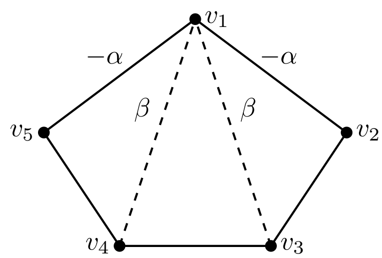

FIG. 4. *The cycle graph on five vertices C_5. Coupling strengths for the vertex v_1 are displayed.*

For the current scheme of coupling in graph C_5, due to the topology of the graph the vertex v_1 is free to synchronize with vertices v_3 and v_4. However since the coupling strength is equal (β in both cases), the vertex doesn't synchronize with either v_3 or v_4. By the symmetry in the topology of the graph, the argument remains same if v_1 is replaced by any other vertex. Thus we observe that upon coupling Thomas' system under the scheme given in Equation 3.5 for graph C_5, all the oscillators representing the vertices converge to different coordinates over time and none synchronize with any other.

To overcome the limitations in finding optimal graph colouring imposed by symmetry in coupling strength, we consider a different scheme for coupling oscillator systems such that the coupling strengths are varied or asymmetric. In order to achieve the same, instead of assigning the same value (α or β) of coupling strength, we order the number of edges and non-edges i.e pair of vertices between which there is no edge (except for self-loops), and add an incremental constant to the initial value of coupling strength whenever a new edge or non-edge is encountered. That is to say if number of edges in a given simple graph G are p and thus number of non-edges i.e. pair of vertices without an edge or a self loop between them are $\binom{n}{2} - p - n = q$, then the coupling equations can be represented as

$$\dot{u}_i(t) = f_{u_i}(x, y, z) + \sum_{j=1, j\neq i}^{N} K_{ij} \frac{(u_i(t) - u_j(t))}{(1 + (u_i(t) - u_j(t))^2)} \tag{3.7}$$

where $K_{ij} = -(\alpha + kc_1)$ for the k^{th} edge such that $0 \leq k \leq p-1$ and $K_{ij} = \beta + lc_2$ for the l^{th} non-edge such that $0 \leq l \leq q-1$.

A simple way to find such an asymmetric coupling matrix given the adjacency matrix A for the graph is to traverse the upper triangular indices of A and incrementally assign value $-(\alpha + kc_1)$ in the K_{ij} and K_{ji} index whenever a 1 is encountered and $\beta + lc_2$ whenever 0 is encountered. Thus for example the coupling matrix K_{C_5} for the choice of constants α, β, c_1 and c_2 as 10, 1, 0.25 and 0.1 for the graph C_5 shown in Figure 4 becomes

$$K_{C_5} = \begin{pmatrix} 0 & -10 & 1 & 1.1 & -10.25 \\ -10 & 0 & -10.50 & 1.2 & 1.3 \\ 1 & -10.50 & 0 & -10.75 & 1.4 \\ 1.1 & 1.2 & -10.75 & 0 & -11 \\ -10.25 & 1.3 & 1.4 & -11 & 0 \end{pmatrix}$$

such that

$$A_{C_5} = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

is an adjacency matrix for C_5. A theoretical study of such asymmetric coupling matrices with respect to graph coloring may be considered interesting by mathematicians and data scientists alike and may open an avenue for further research.

For the current study, it can be observed that since the Runge-Kutta (RK4) method we are using is linear in time and as can be observed from the equation 3.7, the method runs for $3n$ instances, separately for each coordinate, for a graph of order n. Also one can notice that the equation form presented in equation 3.7 is dependent on n, as the calculations made for each coordinate are in the order of n for a given iteration. Thus if t is the length of the time interval for which the method runs in order to infer synchronization in different coupled oscillators, the overall time complexity of the procedure thus becomes $O(n^2t)$.

Coupling the Thomas' system using asymmetric coupling as described here substantially improves finding optimal graph colouring for different graphs. For instance, for the choice of parameters α, β, c_1 and c_2 described in Equation 3.7 as 15.75, 5, 1 and 0.5 respectively, we find that all connected graphs of order 5 except the *kite* graph (also called $co-fork$ or $co-chair$) and $5-cycle$ or C_5 show optimal graph colouring. Furthermore, these graphs, *kite* graph and C_5 show optimal graph colouring for the chouce of parameters α, β, c_1 and c_2 as 8, 1.5, 1 and 0.5 respectively. For the choice of parameters α, β, c_1 and c_2 as 8, 1.5, 1 and 0.5 respectively, all connected graphs of order five except the *house* graph (i.e., $\overline{P_5}$) and the graph $\overline{claw \cup K_1}$ show optimal graph colouring when Thomas' systems are coupled as per the scheme described in Equation 3.7.

It must be noted that for a given coupled system, the synchronization in oscillators under the proposed scheme is dependent on the initial values of the coordinates chosen for the oscillators and for the same choice of parameters, the coupled system may or may not show synchronization based on difference in the initial values. In particular, in the present work, the initial value for all the oscillators are set to zero (i.e, all oscillators lie at origin in the beginning) except for one such oscillator whose initial values (in one of the coordinates) is slightly perturbed.

3.3. Dependence of Graph Colouring on Parameters α and β. As is clear from the results for asymmetric coupling in graphs of order five, a particular choice of parameters α, β, c_1 and $c_2 2$ may not return optimal graph colouring for all connected graphs of a given order. Thus we wish to find if there exist a universal choice of parameters α ad β or a particular ratio of these values $\frac{\alpha}{\beta}$ that return optimal graph colouring for all connected graphs when coupled asymmetrically for a fixed choice of parameters c_1 and c_2 and a given set of initial conditions.

Thus in order to analyse the role of the parameters α and β in producing optimal colouring classes upon synchronization in asymmetrically coupled oscillators, we choose to vary α and β for a fixed choice of parameters c_1 and c_2 and given initial condition. We arbitrarily choose some graphs from the list of small (of order up to six) connected graphs and initially choose to vary α from n to n^2, and β from 1 to n, where n is the order of the chosen graph. We find that for the choice of c_1 and c_2 respectively as 1 and 0.5, some graphs, for instance, the graph P_3 and $4-\textit{cycle}$ i.e., P_4, produce optimal graph colouring upon asymmetric coupling for all values of parameters α and β varied in the given range. The results are summarized as Figure 5, where we assign cyan colour for the given choice of α and β varied in range n to n^2 and 1 to n respectively, if optimal colour classes are obtained upon synchronization when Thomas' systems are coupled asymmetrically.

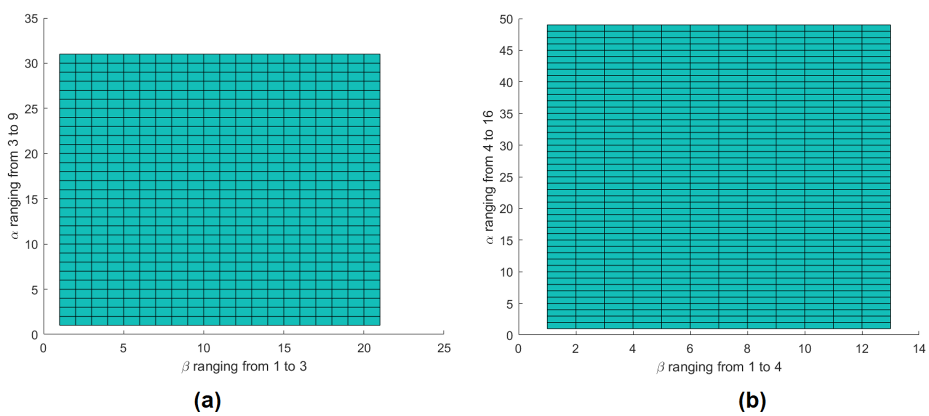

FIG. 5. *Graph colouring for asymmetrically coupled Thomas' systems for the graphs (a) P_3 and (b) C_4. The optimal graph colour classes for the choice of parameters α and β is shown in cyan colour.*

It is however observed that when we vary α and β in the range n to n^2 and 1 to n respectively as described earlier, most graphs tend to return optimal graph colouring upon synchronization in asymmetrically coupled Thomas' systems for a certain values of the parameters α and β, while for other values the graph classes returned upon synchronization are sub-optimal. The data presented as Figure 6 summarize the results obtained for some graphs of order four to six, when the parameters α and β are varied in the range n to n^2 and 1 to n respectively. Optimal graph colour classes obtained upon synchronization for the given choice of parameters α and β is shown in blue colour, while the sub-optimal colour classes is shown in yellow colour.

It is clearly observed from the results presented in the Figure 6 that the range of parameters α and β such that optimal graph colouring is obtained as a result of asymmetrically coupling Thomas' systems in the given range, is completely dependent on the topology of the underlying graph. Thus it may not be possible to find universal values of α and β or a ratio thereof of these parameters that return optimal graph colouring irrespective of the graph used for coupling. In turn, this observation lets us to believe that due to the inherent difference in the topology, some graphs are

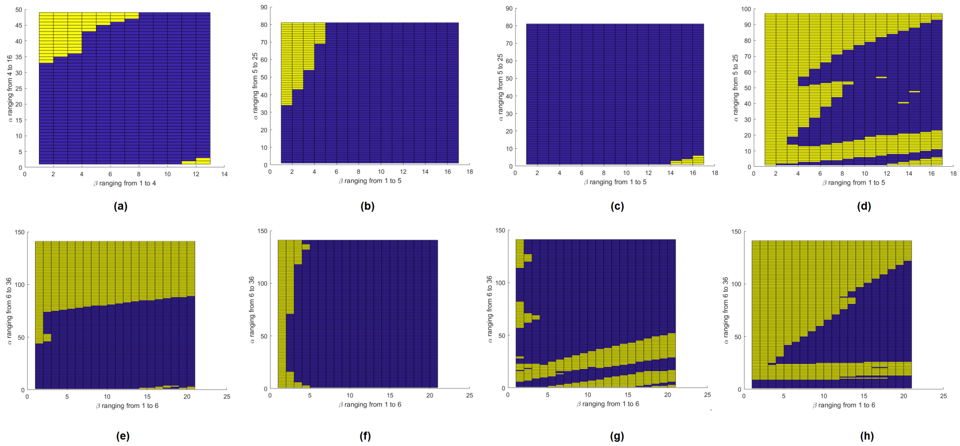

FIG. 6. *Graph colouring for asymmetrically coupled Thomas' systems for the graphs (a) paw or* $3-pan$*, (b) bull, (c) cricket or* $K_{1,4}+e$*, (d)* $\overline{P_2 \cup P_3}$*, (e)* $\overline{H}$*, (f)* $\overline{X_{18}}$*, (g)* $\overline{X_{37}}$ *and (h)* $\overline{X_{197}}$*. The optimal graph colour classes for the choice of parameters* α *and* β *is shown in blue colour. The boxes shown in yellow colour show sub-optimal colour classes obtained upon synchronization in asymmetrically coupled Thomas' systems for the choice of parameters* α *and* β*.*

more susceptible to showing optimal graph colouring when oscillators are coupled asymmetrically as per the topology of these graphs.

We further observe that for some graphs, the choice of parameters α and β may produce an invalid graph colouring in asymmetrically coupled oscillators i.e., some adjacent vertices in the graph are assigned the same colour classes upon synchronization. The following results obtained for graphs of order six X_{96} and $\overline{X_{172}}$, presented here as Figure 7, showcase these observations.

3.4. Dependence of Graph Colouring on Parameters c_1 and c_2. Having studied the role of parameters α and β on graph colouring in asymmetrically coupled Thomas' systems, we now intend to focus on the role of the parameters c_1 and c_2 in the vicinity of an optimal solution. That is to say, if we obtain an optimal solution for a particular choice of parameters α and β for a given choice of parameters c_1 and c_2, then we wish to study whether what are the implications of varying c_1 and c_2 in such a scenario. Thus in some sense we enquire into the nature of overall stability of the optimal solutions, given the parameters α, β c_1 and c_2.

We arbitrarily choose three different graphs of order six, namely $\overline{H}, \overline{X_{172}}$ and $\overline{X_{197}}$ and vary the parameters c_1 and c_2 for three different choices of parameters α and β for each graph. We first vary parameters c_1 and c_2 over a range varying from 0.4 to 1.6 and 0.1 to 0.9 respectively with an increment of 0.05 in each case. Upon varying the parameters c_1 and c_2 over this small range for the three different choices of graphs, it is observed that whether optimal graph colouring is returned upon asymmetric coupling in a graph as previously described depends completely on the topology of the graph. Moreover, it is observed that for a given graph, different choices of parameters α and β, returns different ranges of parameters c_1 and c_2 for which an optimal graph colouring is observed upon asymmetric coupling of Thomas' systems. These observations are summarized as Figure 8 and Figure 9.

We further vary parameters c_1 and c_2 over a larger range i.e. from 1 to 25 and 1 to

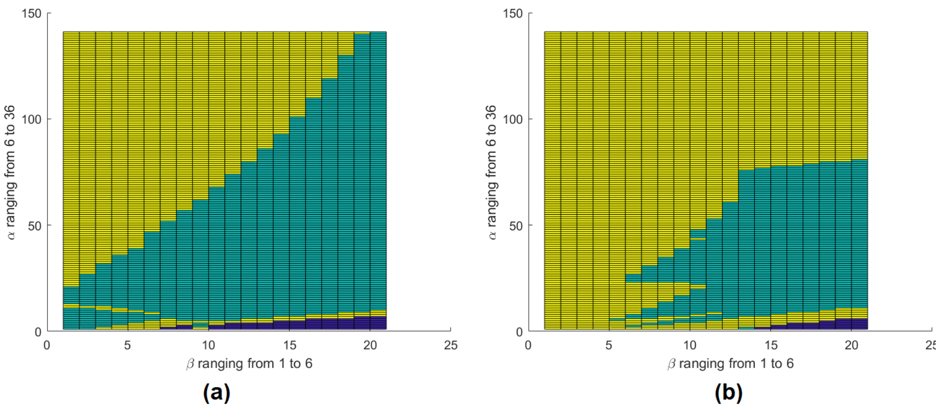

FIG. 7. *Graph colouring for asymmetrically coupled Thomas' systems for the graphs (a) X_{96} and (b) $\overline{X_{172}}$. The optimal graph colour classes for the choice of parameters α and β is shown in cyan colour. The boxes shown in yellow colour show sub-optimal colour classes obtained upon synchronization in asymmetrically coupled Thomas' systems for the choice of parameters α and β. The area in blue represents the range of parameters α and β which return invalid graph colouring upon synchronization.*

17 respectively, for the same choices of parameters α and β in the graphs considered previously. It is observed that when we vary c_1 and c_2 over a large range of values while keeping the values of parameters α and β as fixed, the fact that optimal graph colouring is returned as a result of asymmetric coupling based on a given graph is dependent on the topology of the graph. As can be seen from results shared as Figure 10, for some graphs such as $\overline{H}$, optimal graph colouring can be found for even very large values of the parameters c_1 and c_2. While for some other graphs, for instance the graph $\overline{X_{172}}$, optimal graph colouring is returned only for small values of parameters c_1, while the results seem independent of c_2.

It can be further observed with the help of Figure 11, that for some graphs we may obtain invalid graph colouring for some choices of parameters c_1 and c_2, while the parameters α and β are fixed. Thus we observe that the particular topology of the graph has a dominant role in determining if an optimal graph colouring is returned as a result of coupling Thomas' systems asymmetrically based on some graph.

3.5. Graph Colouring in Larger Graphs. At this point we wish to make an important observation on the nature of synchronization in asymmetrically coupled systems, as a function of order n of the underlying graph. It is observed that graphs of small order show a good synchronization, in the sense that the Euclidean distance between the coordinate values of the synchronized oscillators is nearly zero. However, as the order of the underlying graph (based on which the couplings are made in the system of oscillators) is increased, it is observed that the Euclidean distance between coordinates of some of the synchronized oscillators is more than the coordinate distance between other synchronized oscillators. However, this increased distance is still far less than the Euclidean distance between coordinates of oscillators that have not synchronized. We demonstrate these observations with the help of data presented here as table 2.

As the distance between coordinate values of synchronized oscillators is quite

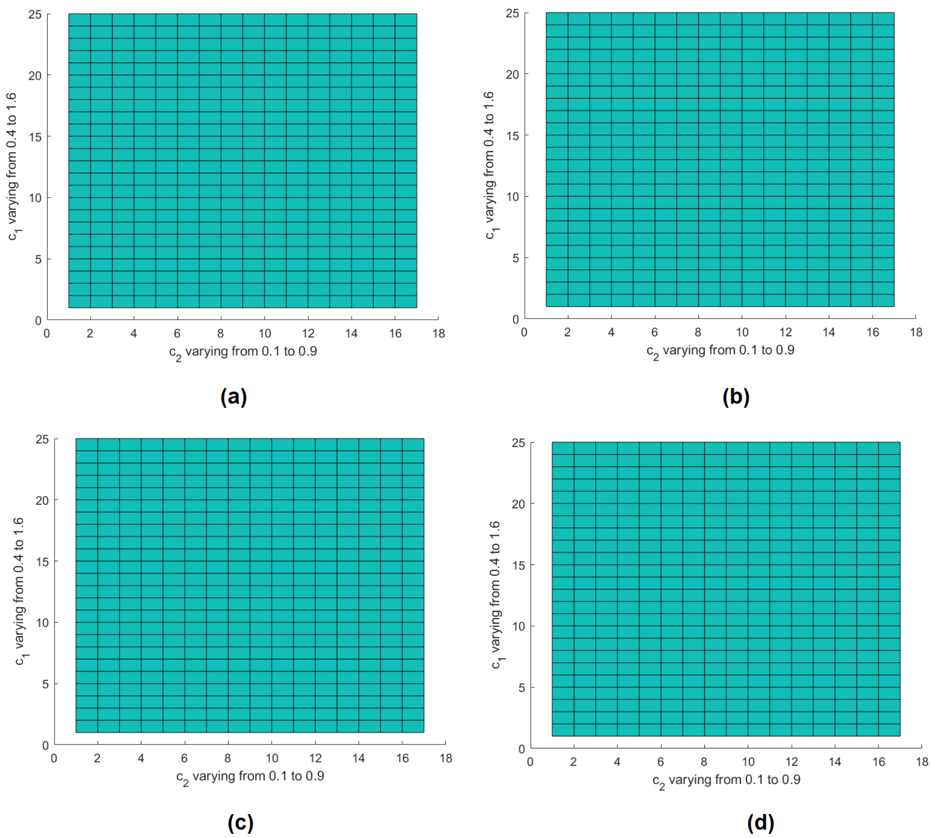

FIG. 8. *Graph colouring for asymmetrically coupled Thomas' systems for a fixed choice of parameters* α *and* β *and varying* c_1 *and* c_2 *over a small range, 0.4 to 1.6 and 0.1 to 0.9 respectively. Optimal colour classes are obtained (shown in cyan colour) over over the entire range for (a)* $\overline{H}$ *and* $\alpha = 9.5$ *and* $\beta = 2$*, (b)* $\overline{H}$ *and* $\alpha = 10.75$ *and* $\beta = 3.25$*, (c)* $\overline{X_{172}}$ *and* $\alpha = 13.25$ *and* $\beta = 4.5$ *and (d)* $\overline{X_{172}}$ *and* $\alpha = 15.75$ *and* $\beta = 5.75$*.*

small in graphs of small order, it is easy to consider a small threshold value of the Euclidean distance (say 1) such that oscillators with distance between coordinates below this threshold value are considered in the same colour class and those above the threshold values are considered as belonging to different colour classes. However, as the order of the graph increases and hence the Euclidean distance between coordinates of synchronized oscillators increases in many cases, it becomes difficult to find such a threshold value of distance. In order to mitigate this problem, we assume that the coordinate distances between synchronized oscillators must follow a normal distribution and the values of coordinate distance for oscillators that have not synchronized with a given set of oscillators will fall away (in terms of Z-score) from this normal distribution of coordinate distances between synchronized oscillators.

Thus in order to find the maximum distance between the coordinate values of any two oscillators that have synchronized (for graphs of order greater than six), we start with an array of sorted coordinate distances between different oscillators and

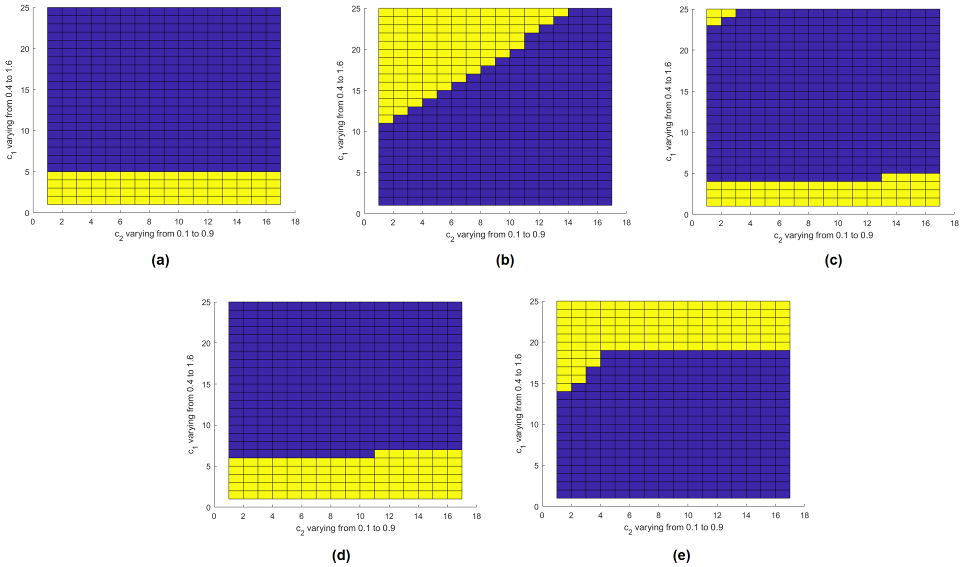

Fig. 9. *Graph colouring for asymmetrically coupled Thomas' systems for a fixed choice of parameters α and β and varying c_1 and c_2 over a small range, 0.4 to 1.6 and 0.1 to 0.9 respectively. Optimal colour classes are shown in blue colour, while sub-optimal colour classes are displayed in yellow for (a) $\overline{H}$ and $\alpha = 15.5$ and $\beta = 4.5$, (b) $\overline{X_{197}}$ and $\alpha = 8.25$ and $\beta = 2$, (c) $\overline{X_{197}}$ and $\alpha = 10.75$ and $\beta = 3.75$, (d) $\overline{X_{197}}$ and $\alpha = 13.25$ and $\beta = 4.75$ and (e) $\overline{X_{172}}$ and $\alpha = 8.25$ and $\beta = 3.75$.*

calculate mean and standard deviation for first k values (starting from k equal three). We then calculate the Z-score:

$$Z_{k+1} = \frac{d_{k+1} - \overline{d_k}}{s_k}$$

where d_{k+1} is the $k+1^{th}$ smallest distance, $\overline{d_k}$ is the mean of the first k smallest distances and s_k is the standard deviation of the first k smallest distances. If we find that the Z-score is larger than a threshold value (say 6), then we consider d_k, the k^{th} smallest distance as the maximum distance between coordinate values of synchronized oscillators. Once we have established the maximum distance hence, we consider all the oscillators with mutual coordinate distance below this maximum value to belong to the same colour class.

We make use of the method based on Z-score to find the range of parameters α and β for a fixed choice of parameters c_1 and c_2, such that optimal graph colouring is returned upon asymmetric coupling Thomas' systems for a graph of order eight. The graph of order eight (which is not named in the ISGCI system) and the results based on varying the parameters α and β for the given graph are presented here as Figure 12. The method based on Z-score successfully identifies the maximum coordinate distance between synchronized oscillators in most cases, however, in some cases it fails to do so. For the results presented here as Figure 12, the sub-optimal graph colouring obtained for lower values of α and higher values of β (seen as thin yellow area sandwiched

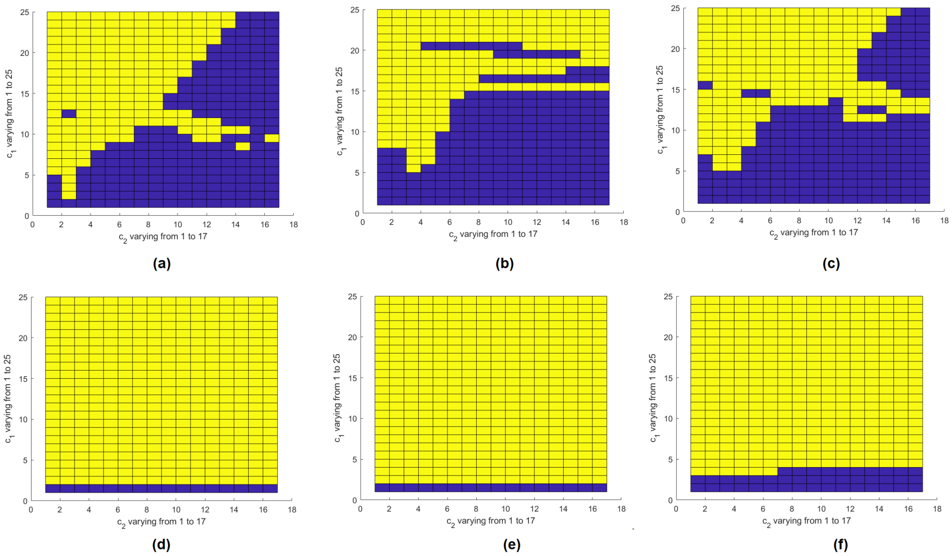

Fig. 10. *Graph colouring for asymmetrically coupled Thomas' systems for a fixed choice of parameters α and β and varying c_1 and c_2 over 1 to 25 and 1 to 17 respectively. Here (a), (b) and (c) are graph colourings obtained by varying c_1 and c_2 for the order 6 graph $\overline{H}$ for choice of α and β for (a) being 9.5 and 2, (b) being 15.5 and 4.5 and (c) being 10.75 and 3.25. The boxes in yellow show sub-optimal graph colouring and the boxes in blue correspond to values of c_1 and c_2 for which optimal graph colouring is obtained. Similarily, in (d), (e) and (f) we have results for the graph $\overline{X_{172}}$, for choice of α and β being for (d) 8.25 and 3.25, for (e) 13.25 and 4.5 and for (f) 15.75 and 5.75.*

between blue region representing invalid graph colouring) is due to error in the method while identifying the maximum coordinate distance between synchronized oscillators.

We further observe that for a fixed value of the parameter β, given a graph G, the number of colour classes usually increases as the value of α is increased (from invalid, i.e less than χ_G to optimal to sub-optimal with increasing number of colour classes). We make use of this fact to come up with a simple way to find optimal graph colouring in larger graphs (given that χ_G is known) by guessing an appropriate value of the parameter β and reducing or increasing the value of α for the given choice of β depending on whether the obtained graph classes for a choice of α are sub-optimal with high number of colour classes or invalid colouring with number of colour classes less than the chromatic number.

We try to find the graph colouring for some graph-vertex colouring instances that are commonly used in the literature (a list of such instances can be found at https://sites.google.com/site/graphcoloring/vertex-coloring). However it is found that for the exception of relatively small graphs myceil3 and myceil4 of order 11 and 23 respectively (results shared as Table 2), parameters corresponding to optimal graph colouring could not be found for such benchmark graphs. It is rather observed that for these benchmark graphs the method produces invalid colouring of the same sizes as the optimal graph colouring for different choices of parameters α, β, c_1 and c_2.

Thus we wish to understand the reasons due which the method fails to generate optimal graph colouring for larger benchmark graphs. In particular, we wish to un-

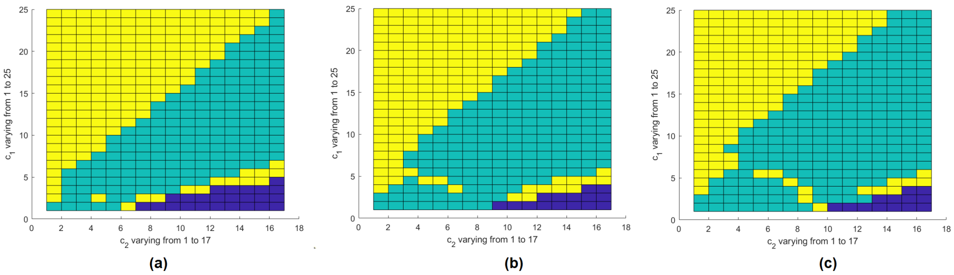

FIG. 11. *Graph colouring for asymmetrically coupled Thomas' systems for a fixed choice of parameters α and β and varying c_1 and c_2 1 to 25 and 1 to 17 respectively. Here (a), (b) and (c) are graph colourings obtained by varying c_1 and c_2 for the order 6 graph $\overline{X_{197}}$ for choice of α and β for (a) being 8.25 and 2, (b) being 10.75 and 3.75 and (c) being 13.25 and 4.75. The boxes in yellow show sub-optimal graph colouring, while the boxes in cyan show optimal graph colouring. The boxes in blue correspond to values of c_1 and c_2 for which invalid graph colouring is obtained.*

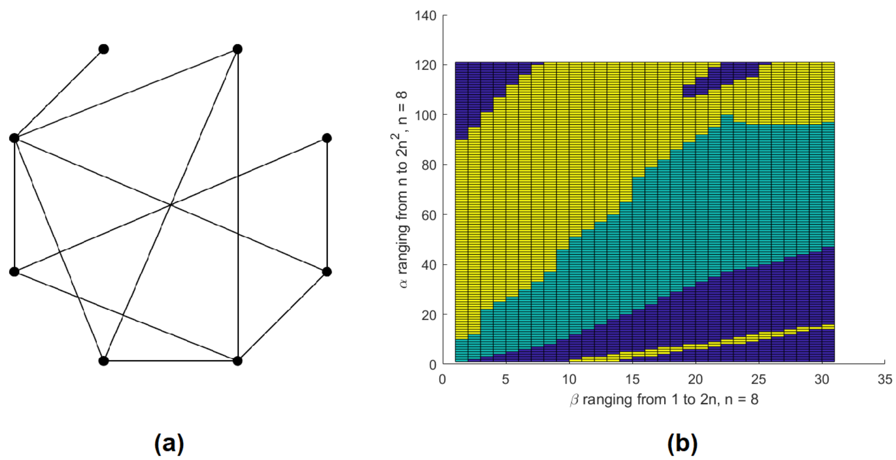

FIG. 12. *Graph colouring for asymmetrically coupled Thomas' systems for a graph G of order eight. (a) The graph G and (b) the results of graph colouring for graph G. The optimal graph colour classes for the choice of parameters α and β is shown in cyan colour. The boxes shown in yellow colour show sub-optimal colour classes obtained upon synchronization in asymmetrically coupled Thomas' systems for the choice of parameters α and β. The area in blue represents the range of parameters α and β which return invalid graph colouring upon synchronization.*

derstand if the method returning an optimal graph colouring for some choice of the parameters α, β, c_1 and c_2 is purely dependent on the size of the graph in question or is somehow dependent on the topology of the particular graph in question. In order to answer the question, we try to find the optimal graph colouring in some graphs with simplest possible topologies. For instance, we consider the star graphs ($K_{1,n}$, the complete bipartite graph with one of the partition containing a single vertex), path graphs and cycles (while considering that the topologies of odd and even cycles are different, even cycles being bipartite graphs) and try to come up with optimal graph colouring for these graphs by varying their order and sizes.

It is observed that for some graphs with specific topology like the star graphs (or $K_{1,n}$), the method easily finds the optimal graph colouring for graphs of even large order and sizes (as seen in results shared as Table 2). However, for other topologies the method fails to produce optimal graph colouring for choice of parameters α, β, c_1 and c_2. For instance, the method fails to produce optimal graph colouring and returns an invalid graph colouring of size 3 and 2 respectively for cycle and path of order 19 and 21 respectively, while it produces valid optimal graph colouring for subsequently smaller sizes. Thus we observe that both the topology of the graph and the order and size of the graph play a role in determining if the method returns an optimal graph colouring for some choice of parameters α, β, c_1 and c_2 and as the complexity of the graph increases with the increase in the order and size of the graph, the method ceases to return an optimal graph colouring.

Conclusions. The present study presents a very peculiar and novel approach to study graph colouring where oscillators are coupled negatively or positively, which respectively represent the repulsive and attractive forces in nature and the oscillators coupled on the basis of an underlying graph produce synchronization in these oscillators in such a way that the oscillators corresponding to those vertices in the graph which should lie in the same colouring class, synchronise. It is observed that oscillators such as Thomas' system with a relatively simple set of equations are best suited for the purpose.

We further conclude that one must introduce asymmetry in coupling forces in the form of variation in coupling strengths so that the effects of symmetry in the topology of the graph that hinders the synchronization in oscillators to produce optimal graph colouring is countered in some graph.

We further studied the role of coupling parameters α, β, c_1 and c_2, encountered as a result of the asymmetric coupling equations, in producing optimal graph colouring upon synchronization. We find that the choice of parameters α, β, c_1 and c_2 that produce optimal graph colouring for a given graph is dependent on the topology of the graph. It is further observed that for a fixed choice of parameter β, increasing the value of parameter α is likely to produce an invalid graph colouring, followed by optimal colouring and produces a sub-optimal graph colouring for further increase in the value of α for an arbitrary graph.

In the present study, it is further noticed that the polynomial time method developed in this study produces optimal graph colouring for all classes of graphs up to a certain order and size. However, as the order and size and hence the resultant complexity of the graph increases depending on the topology of the graph, the method ceases to produce optimal colour classes. It must be noted however that for few topologies like star graphs ($K_{1,n}$), the method produces optimal colour classes for a large value of order and size of the graph. Thus synchronization under the defined conditions is favoured by the star topology.

The present work discusses the emergence of optimal graph colouring as a result of coupling oscillators with varying degree of attraction and repulsion between the agents. Since graph colouring is an example of a hard-problem encountered while solving numerous real-life problems (for instance, travelling salesman problem as encountered during logistic implementation of supply-chain processes), the work presents an insightful understanding of how natural agents or processes may deal with such problems using some simple rule based approaches based on attraction-repulsion pairings. We further conclude that success in achieving solutions to such hard-problems shall depend on the topology, i.e., on the exact nature of interaction between different agents present in the system and that such solutions may only emerge for problems up-to a certain size, that is to say for up-to a certain number of agents, while for agent interactions following certain typologies (star topology for example), the solutions may readily emerge even for large number of agents in the system.

Finally, we wish to conclude that graph colouring is studied here in a complex adaptive dynamical systems framework which produces new and valuable insights into the dependence of synchronization in network of oscillators based on the topology of the underlying graphs. The limitations of methodology presented in the current study open further avenues of research into this area and theoretical advancements that may be made in order to overcome these limitations shall produce a valuable resources of scientific knowledge and understanding in future.

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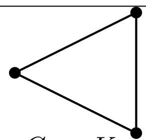
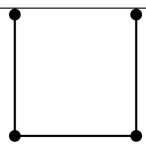
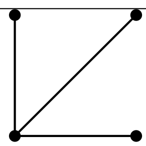
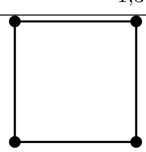
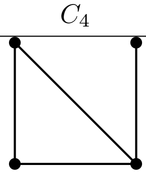
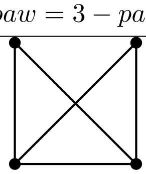
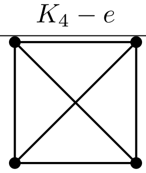
Graph	Chua's Oscillator	Thomas' System	$\dot{u} = -cu$	$\dot{u} = \frac{-cu}{1+u^2}$
 $C_3 = K_3$	3(O)	3(O)	3(O)	3(O)
 P_4	4(SO)	4(SO)	4(SO)	4(SO)
 $claw = K_{1,3}$	2(O)	2(O)	2(O)	2(O)
 C_4	2(O)	2(O)	2(O)	2(O)
 $paw = 3 - pan$	2(W)	2(W)	2(W)	2(W)
 $K_4 - e$	3(O)	3(O)	3(O)	3(O)
 K_4	3(W)	3(W)	3(W)	3(W)

TABLE 1

Graph colouring for choice of different oscillator systems and equations for connected graphs upto order four. The number indicates the graph colouring returned for the given graphs by different systems. O inside parenthesis indicates that the returned graph colouring is optimal, while SO indicates that its sub-optimal but a valid graph colouring. W in parenthesis indicates that the graph colouring returned by the system upon coupling is an invalid graph colouring.

Graph	Order of the graph	Number of edges	Parameter values for optimal graph colouring
myceil3	11	20	$\alpha = 80$, $\beta = 10$, $c_1 = 1$ and $c_2 = 0.75$
myceil4	23	71	$\alpha = 190$, $\beta = 20$, $c_1 = 1$ and $c_2 = 0.5$
$K_{1,29}$	30	29	$\alpha = 260$, $\beta = 28$, $c_1 = 1$ and $c_2 = 0.5$
$K_{1,59}$	60	59	$\alpha = 480$, $\beta = 58$, $c_1 = 1$ and $c_2 = 0.5$
$K_{1,89}$	90	89	$\alpha = 810$, $\beta = 88$, $c_1 = 1$ and $c_2 = 0.5$
$K_{1,119}$	120	119	$\alpha = 1150$, $\beta = 116$, $c_1 = 1$ and $c_2 = 0.5$

TABLE 2
Parameter values corresponding to optimal graph colouring for graph of different order and sizes.