

2 *Supplementary Material*

S1 ADDITIONAL TABLES AND FIGURES REFERENCED IN THE MANUSCRIPT

Parameter	Value
a	0.7
b	0.8
τ	12.5
$\bar{g}_{coup}$	{varies}

Table S1. Parameter values of the FHN model.

Parameter	Value	Parameter	Value	Parameter	Value
C_m (fF)	5310	V_m (mV)	4	S_m (mV)	14
V_n (mV)	-15	S_n (mV)	5.6	κ_1 (mV)	65
κ_2 (mV)	20	$\bar{\tau}$ (ms)	37.5	$\bar{V}$ (mV)	-75
V_h (mV)	-10	S_h (mV)	-10	$\bar{g}_K$ (pS)	2500
$\bar{g}_{Ca}$ (pS)	1400	V_K (mV)	-75	V_{Ca} (mV)	110
K_d (μ M)	100	$\bar{g}_{K-Ca}$ (pS)	30000	f	0.001
k_{Ca} (ms^{-1})	0.03	$\alpha \left(\frac{\mu\text{m}^3 \text{Coul}}{\text{mMol}} \right)$	4.5061×10^{-6}	$\bar{g}_{coup}$ (pS)	{varies}

Table S2. Parameter values of the SRK model.

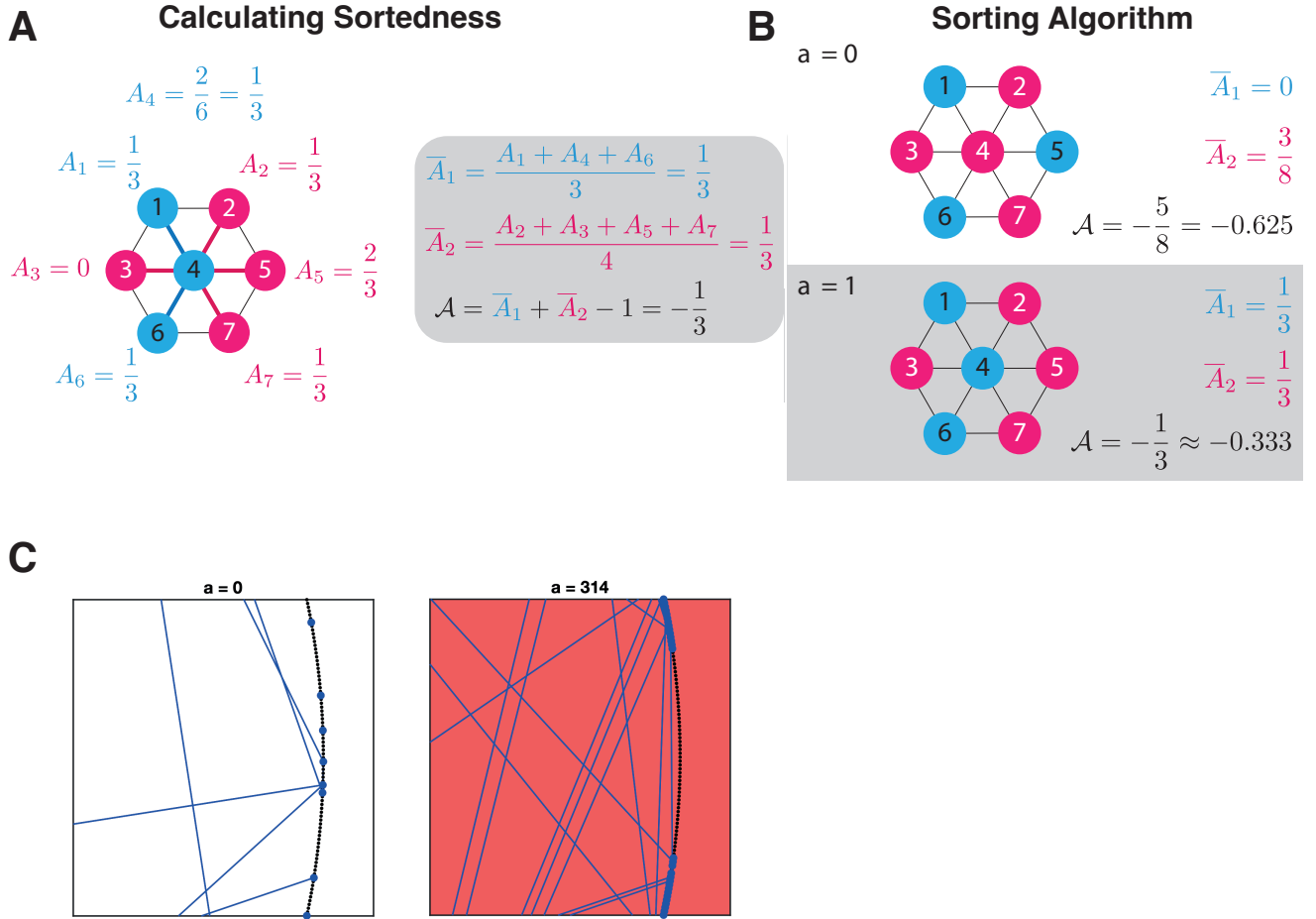


Figure S1. Sortedness and the sorting algorithm. **A.** An illustration of node, population, and network sortedness calculations on a small network. **B.** A successful iteration of the forward sorting algorithm. **C.** These are zoomed in portions of the WS networks, which are shown as black boxes in Fig. 2A. The initial network ($a = 0$) shows the population 1 nodes mostly isolated, but the final network ($a = 314$) shows two distinct clusters of several population 1 nodes.

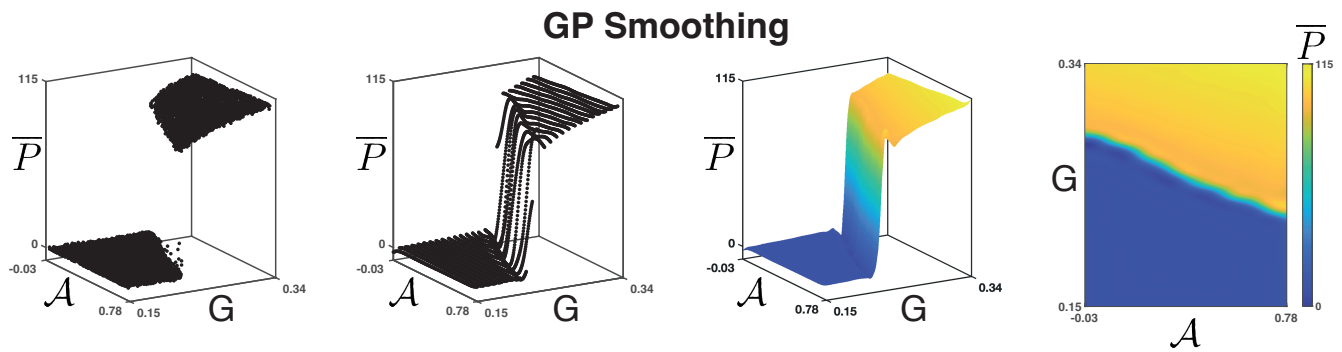


Figure S2. Gaussian process regression model. We now simulate dynamics on networks where (G, a) pairs are selected on a Latin hypercube. For each point, we use a different initial network P_k^0 and run the sorting algorithm to find the network P_k^a . We also use randomly selected initial conditions, $Y(0)$. In the case of the WS networks, we also use a different WS graph for each point. *Left panel* The feature $\bar{P}$ is shown as a scatter plot for each point $(G, \mathcal{A})$. *Middle-left panel* We use a Gaussian process regression model trained to the data on the Latin hypercube to estimate the points on a regular grid. *Middle-right panel* We can use this smoothed dataset to produce surface plots. *Right panel* We show the panels as heatmaps. Here, we show the resulting heatmap after training GP model with 10000 points using the WS-FHN network model. This is for the case where coupling is strong ($\bar{g}_{coup} = 0.1$).

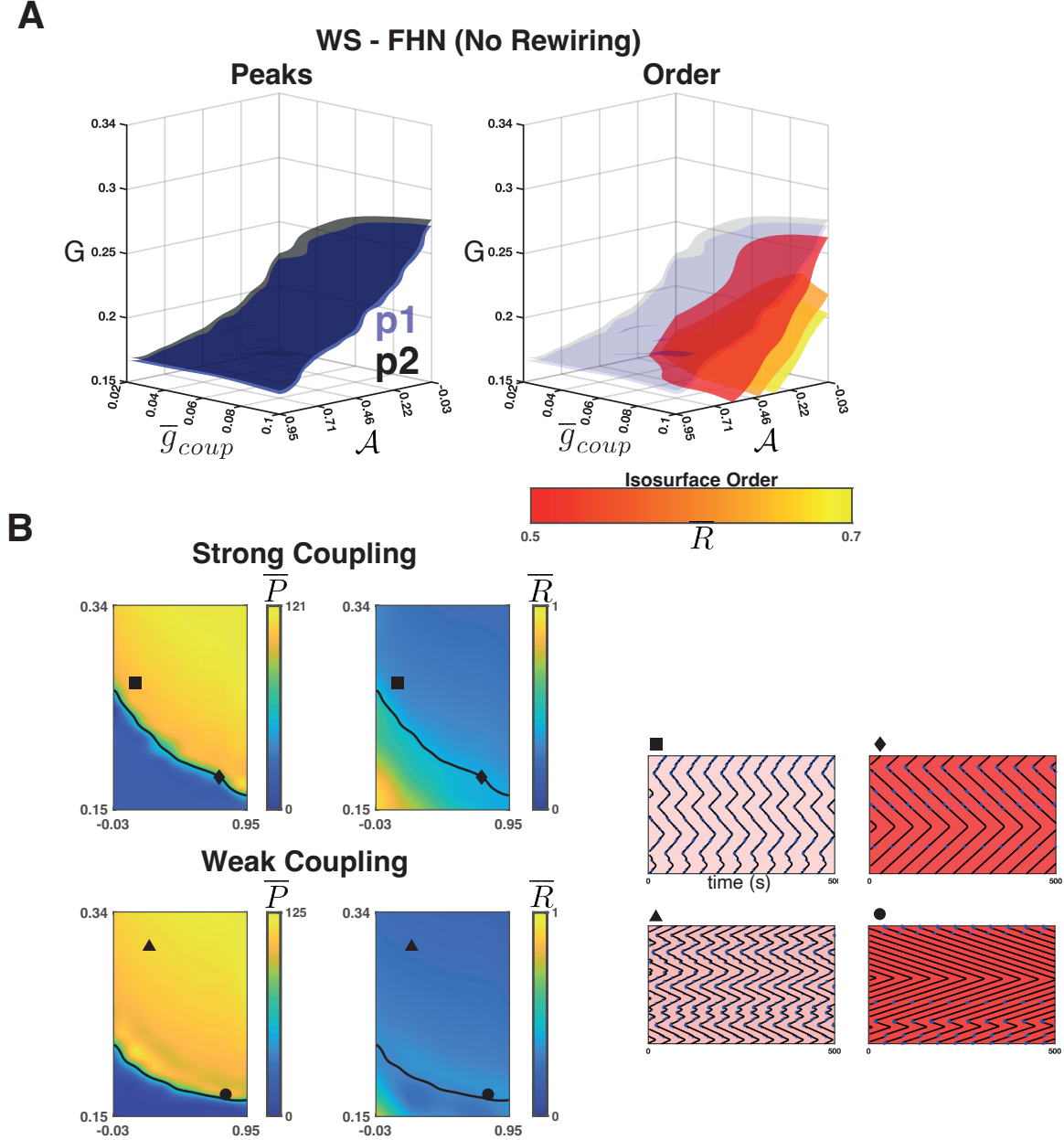
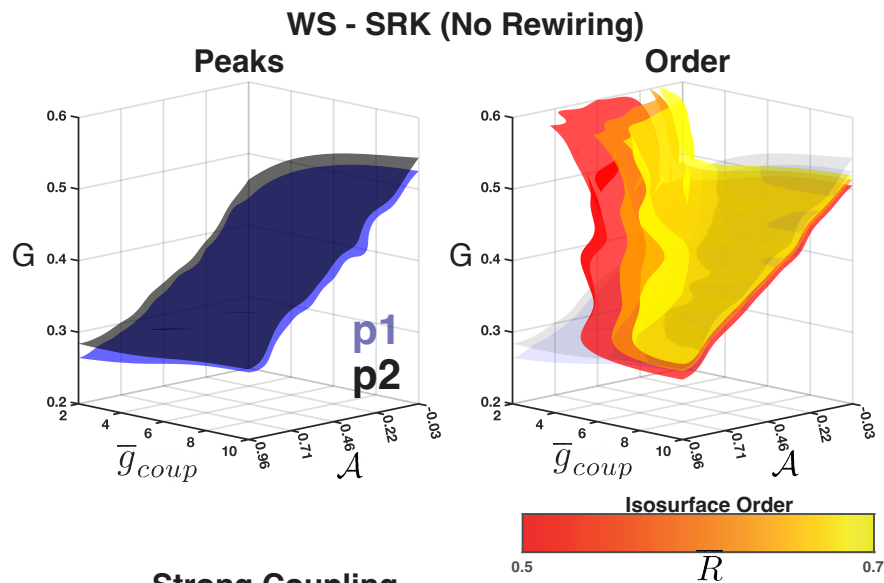


Figure S3. No rewiring in the WS-FHN networks. **A. Left panel:** The isosurfaces for the $\bar{P}_1$ (blue) and $\bar{P}_2$ (black) half-maxima in the WS-FHN networks with no rewiring. These surfaces do not separate. **Right panel:** The isosurfaces for $\bar{R}$ illustrate the boundary between low and high synchrony as well as its direction in the WS-FHN, $\beta = 0$ networks. Within the active region, synchrony is always low due to the propagation of waves. **B.** Heatmaps for $\bar{P}$ (top left panel) and $\bar{R}$ (top right panel) when $\bar{g}_{coup} = 0.1$ (strong). Heatmaps for $\bar{P}$ (bottom left panel) and $\bar{R}$ (bottom right panel) when $\bar{g}_{coup} = 0.02$ (weak). This shows that the phase transition is still a decreasing function of $\mathcal{A}$, but that synchrony is low regardless of coupling strength. Square, diamond, triangle, and circle show wave propagation for strong and weak coupling and low and high sortedness.

A



B

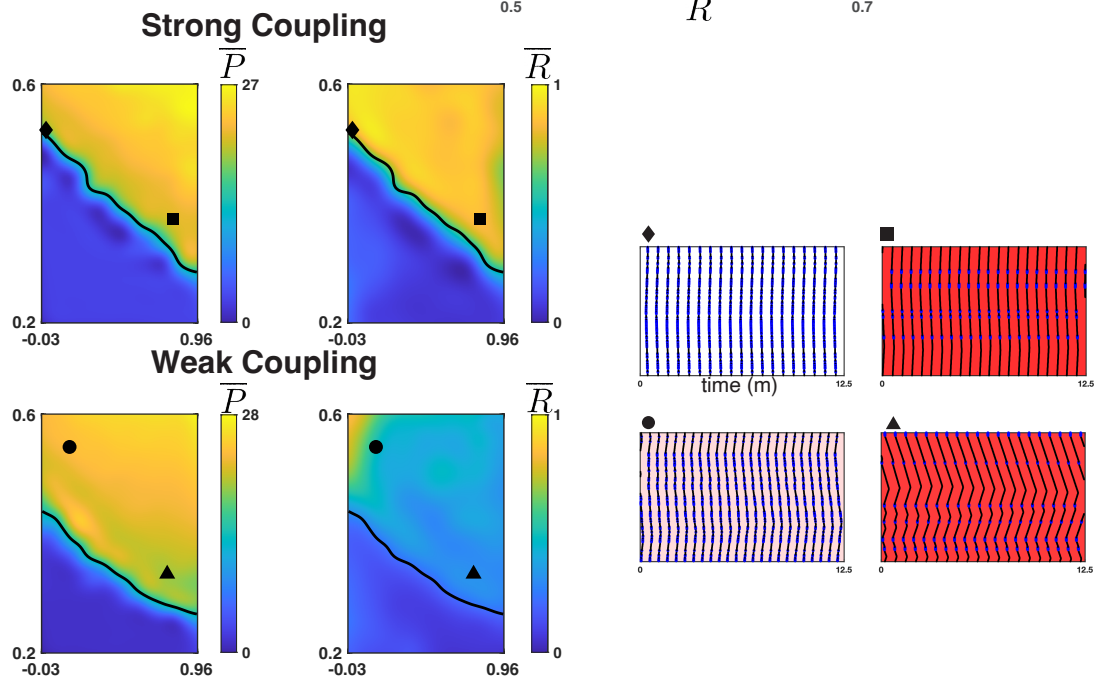


Figure S4. No rewiring in the WS-SRK networks. **A. Left panel:** The isosurfaces for the $\bar{P}_1$ (blue) and $\bar{P}_2$ (black) half-maxima in the WS-SRK networks with no rewiring. These surfaces do not separate. **Right panel:** The isosurfaces for $\bar{R}$ illustrate the boundary between low and high synchrony as well as its direction in the WS-SRK, $\beta = 0$ networks. Within the active region, synchrony is low for low to intermediate coupling due to wave propagation. **B.** Heatmaps for $\bar{P}$ (top left panel) and $\bar{R}$ (top right panel) when $\bar{g}_{coup} = 10$ (strong). Heatmaps for $\bar{P}$ (bottom left panel) and $\bar{R}$ (bottom right panel) when $\bar{g}_{coup} = 2$ (weak). This shows that the phase transition is still a decreasing function of $\mathcal{A}$, that synchrony is low for weak coupling, but that synchrony is still high for strong coupling. *Square* and *diamond* show synchronous activity for strong coupling. *Triangle*, and *circle* show wave propagation for weak coupling, but that the wave propagation remains fast relative to the period of c .

S2 DESCRIPTION OF THE ROUTINES USED TO GENERATE A β C LATTICE NETWORK AND PERFORM THE SORTING ALGORITHM ON IT

Algorithm 2-Algorithm 7 are used by Algorithm 1 which is described in the main text.

Algorithm 2 returns a set of points in $\mathbb{R}^3$ corresponding to the centres of spheres within a hexagonal close packed lattice (hcp). The input r_{ball} corresponds to the radius of the spheres within the lattice, which we set to $r_{ball} = 0.5$ so that the distance between any two nearest neighbors is $d_{ball} = 2r_{ball} = 1$. Algorithm 2 produces the hcp lattice using a sequence of scalings and shifts of a square lattice which takes the points $\{(x, y, z) \mid x, y, z \in \{1, \dots, M\}\}$, where M is an integer corresponding to the number of spheres along the length of the lattice. We sought to embed a larger sphere, S_{net} , of radius R_{net} within the resulting hcp-lattice, and therefore, must choose M such that S_{net} is contained within the lattice. For the square lattice, a natural choice would be $M = 2R_{net}$, so that the length of the lattice equals the diameter of the sphere. However, for the hcp-lattice, the size of the resulting structure is $(M-1)x_{scale} + d_{ball} = Mx_{scale} = Md_{ball}$ by $(M-1)y_{scale} + d_{ball} > My_{scale}$ by $(M-1)z_{scale} + d_{ball} > Mz_{scale}$ (ignoring the shifts). To counteract this, we use:

$$M = \text{ceil} \left(\frac{2R_{net}}{\min([x_{scale}, y_{scale}, z_{scale}])} \right). \quad (\text{S1})$$

We found that this choice of M generated a lattice which could fully embed the sphere, at least for our selection of $R_{net} = 5.55$ (in particular, we increased M and found that the number of nodes within the sphere did not increase).

Algorithm 3 first runs Algorithm 2 to produce an hcp-lattice. It then centres the lattice at the origin (i.e., at $(0, 0, 0)$) and finds all points that are within a sphere of radius R_{net} centred at the origin, which define the nodes in the network. It also returns N , the number of nodes in the spherical hcp-lattice ($N = 1,018$ in this work). Algorithm 4 establishes the Boolean adjacency matrix representing the connections between nodes in the spherical hcp-lattice. A connection exists between two nodes if they are at a distance of d_{ball} from one another. In other words, if two spheres (of radius r_{ball}) centred at the locations assigned to two nodes would be touching, then a connection exists between them. Algorithm 5 determines the population sets P_k for $k \in 1, 2$. It returns the number of nodes N_k in each population, the population membership sets, and the initial network sortedness value A_0 . Algorithm 6 determines the selection probabilities for every pair of nodes ($\{(i, j) \mid i \in P_1, j \in P_2\}$). Algorithm 7 chooses a candidate swap, produces the population sets established by that swap, and calculates $\mathcal{A}$ for the updated population sets.

Algorithm 1 Algorithm for producing networks

Inputs:

N : number of nodes in network

a : number of iterations of swapping algorithm to attempt

Dir : signed integer determining whether algorithm runs forwards (positive) or backwards (negative)

ρ : proportion of population 1 nodes

Outputs:

$\mathcal{A}$: network sortedness value

P_1 : population 1 set

P_2 : population 2 set

n : number of swaps performed

```
1: function GENERATENETWORK( $N, a, Dir, \rho$ )
2:    $(x, y, z), r, K \leftarrow \text{ESTABLISHLATTICE}(N)$ 
3:    $N_1, N_2, P_1, P_2, \mathcal{A} \leftarrow \text{ASSIGNINITIALPOPULATIONS}(N, \rho)$ 
4:    $Term \leftarrow \text{false}$  ▷ Boolean determining whether terminal network state has been reached
5:    $n \leftarrow 0$ 
6:   while ( $n < a$ ) and ( $Term = \text{false}$ ) do
7:      $f, F, Q \leftarrow \text{COMPUTESELECTIONPROBABILITIES}(r[], N_1, N_2, P_1, P_2)$ 
8:      $m \leftarrow 0$ 
9:      $swap \leftarrow \text{true}$  ▷ Boolean determining whether to attempt swaps
10:    while ( $m < N_1 \times N_2$ ) and ( $swap = \text{true}$ ) do
11:       $\tilde{P}_1, \tilde{P}_2, \mathcal{A}_p, k \leftarrow \text{NODESWAP}(f, F, Q, Dir, N_1, N_2, P_1, P_2)$ 
12:      if  $\text{sgn}(\mathcal{A}_p - \mathcal{A}) = \text{sgn}(Dir)$  then
13:         $P_1, P_2 \leftarrow \tilde{P}_1, \tilde{P}_2$ 
14:         $\mathcal{A} \leftarrow \mathcal{A}_p$ 
15:         $n \leftarrow n + 1$ 
16:         $swap \leftarrow \text{false}$ 
17:      else ▷ Reject swap if  $\mathcal{A}$  does not change in the desired direction
18:        for  $l \leftarrow k$  to  $N_1 \times N_2$  do
19:           $F[l] \leftarrow F[l] - f[k]$ 
20:        end for
21:         $Q \leftarrow Q - f[k]$ 
22:         $m \leftarrow m + 1$ 
23:      end if
24:    end while
25:    if  $swap = \text{true}$  then
26:       $Term \leftarrow \text{true}$  ▷ Terminal state has been reached
27:    end if
28:  end while
29:  return  $\mathcal{A}, P_1, P_2, n$ 
30: end function
```

Algorithm 2 Initialising HCP lattice**Inputs:** R_{net} : radius of the spherical lattice r_{ball} : radius of balls around points in the lattice**Outputs:** $(x_1, y_1, z_1), \dots, (x_N, y_N, z_N)$: (x, y, z) coordinates of nodes N : number of nodes in hcp-lattice

```

1: function ESTABLISHHCPLATTICE( $R_{net}, r_{ball}$ )
2:    $d_{ball} \leftarrow 2r_{ball}$ 
3:    $x_{scale} \leftarrow d_{ball}$ 
4:    $y_{scale} \leftarrow \sqrt{d_{ball}^2 - r_{ball}^2}$ 
5:    $z_{scale} \leftarrow \sqrt{\frac{2}{3}}d_{ball}$ 
6:    $x_{shift} \leftarrow r_{ball}$ 
7:    $y_{shift} \leftarrow -\frac{d_{ball}}{\sqrt{3}}$ 
8:    $M \leftarrow \text{ceil}(\frac{2R_{net}}{\min([x_{scale}, y_{scale}, z_{scale}])})$ 
9:    $counter \leftarrow 0$ 
10:  for  $i \leftarrow 1$  to  $M$  do
11:    for  $j \leftarrow 1$  to  $M$  do
12:      for  $k \leftarrow 1$  to  $M$  do
13:         $counter \leftarrow counter + 1$ 
14:         $x[counter] \leftarrow k \times x_{scale}$ 
15:         $y[counter] \leftarrow j \times y_{scale}$ 
16:         $z[counter] \leftarrow i \times z_{scale}$ 
17:        if  $j$  even then
18:           $x[counter] \leftarrow x[counter] + x_{shift}$ 
19:        end if
20:        if  $i$  even then
21:           $y[counter] \leftarrow y[counter] + y_{shift}$ 
22:        end if
23:      end for
24:    end for
25:  end for
26:   $N \leftarrow M^3$ 
27:  return  $(x, y, z), N$ 
28: end function

```

▷ Total number of nodes in the lattice

Algorithm 3 Initialising Sphere lattice

Inputs: R_{net} : radius of the spherical lattice r_{ball} : radius of points in the lattice**Outputs:** $(x_1, y_1, z_1), \dots, (x_{N_{net}}, y_{N_{net}}, z_{N_{net}})$: $(x_{sphere}, y_{sphere}, z_{sphere})$ coordinates of nodes $r_1, \dots, r_{N_{net}}$: r_{sphere} radii of nodes N_{net} number of nodes in the spherical lattice

```
1: function ESTABLISHSPHERELATTICE( $R_{net}, r_{ball}$ )
2:    $(x, y, z), N \leftarrow$  ESTABLISHHCPLATTICE( $R_{net}, r_{ball}$ )
3:    $x \leftarrow x - \text{mean}(x)$  ▷ demean vector x
4:    $y \leftarrow y - \text{mean}(y)$  ▷ demean vector y
5:    $z \leftarrow z - \text{mean}(z)$  ▷ demean vector z
6:    $r \leftarrow \sqrt{x^2 + y^2 + z^2}$  ▷ compute norm over all points
7:    $counter \leftarrow 0$ 
8:   for  $i \leftarrow 1$  to  $N$  do
9:     if  $r[i] \leq R_{net}$  then ▷ Find members of hcp-lattice within sphere radius  $R_{net}$ 
10:       $counter \leftarrow counter + 1$ 
11:       $x_{sphere}[counter] \leftarrow x[i]$ 
12:       $y_{sphere}[counter] \leftarrow y[i]$ 
13:       $z_{sphere}[counter] \leftarrow z[i]$ 
14:       $r_{sphere}[counter] \leftarrow r[i]$ 
15:     end if
16:   end for
17:    $N_{net} \leftarrow counter$  ▷ Define number of nodes within the spherical domain
18:   return  $(x_{sphere}, y_{sphere}, z_{sphere}), r_{sphere}, N_{net}$ 
19: end function
```

Algorithm 4 Initialising lattice

Inputs: R_{net} : radius of the spherical lattice r_{ball} : radius of points in the lattice**Outputs:** $(x_1, y_1, z_1), \dots, (x_N, y_N, z_N)$: (x, y, z) coordinates of nodes $r_1, \dots, r_N$: r radial coordinate of nodes $K \in \mathbb{R}^N \times \mathbb{R}^N$: connectivity matrix

```
1: function ESTABLISHLATTICE( $R_{net}, r_{ball}$ )
2:    $(x, y, z), r, N \leftarrow$  ESTABLISHSPHERELATTICE( $R_{net}, r_{ball}$ )
3:    $d_{ball} \leftarrow 2r_{ball}$ 
4:   for  $i \leftarrow 1$  to  $N$  do
5:     for  $j \leftarrow 1$  to  $N$  do
6:        $dist \leftarrow \sqrt{(x[i] - x[j])^2 + (y[i] - y[j])^2 + (z[i] - z[j])^2}$ 
7:       if  $dist = d_{ball}$  then
8:          $K[i][j] \leftarrow 1$ 
9:       else
10:         $K[i][j] \leftarrow 0$ 
11:      end if
12:    end for
13:  end for
14:  return  $(x, y, z), r, K$ 
15: end function
```

Algorithm 5 Initialising populations

Inputs:

N : number of nodes in network
 ρ : proportion of population 1 nodes

Outputs:

N_1, N_2 : number of nodes in the respective population 1
 P_1, P_2 : population sets
 $\mathcal{A}$: network sortedness

```
1: function ASSIGNINITIALPOPULATIONS( $N, \rho$ )
2:    $U \leftarrow$  random permutation of  $\{1, \dots, N\}$ 
3:    $N_1 \leftarrow \text{floor}(\rho N)$ 
4:    $N_2 \leftarrow N - N_1$ 
5:    $P_1, P_2 \leftarrow$  integer array of length  $N_1$ , integer array of length  $N_2$ 
6:   for  $k \leftarrow 1$  to  $N_1$  do
7:      $P_1[k] = U[k]$  ▷ Assign first  $N_1$  elements of  $U$  to  $P_1$ 
8:   end for
9:   for  $k \leftarrow 1$  to  $N_2$  do
10:     $P_2[k] = U[N_1 + k]$  ▷ Assign last  $N_2$  elements of  $U$  to  $P_2$ 
11:  end for
12:   $\mathcal{A} \leftarrow$  network sortedness value (17) using  $P_1$  and  $P_2$ 
13:  return  $N_1, N_2, P_1, P_2, \mathcal{A}$ 
14: end function
```

Algorithm 6 Defining node pair selection probabilities

Inputs:

$r_1, \dots, r_N$: radial coordinates of nodes
 N_1, N_2 : number of nodes in the respective population
 P_1, P_2 : population sets

Outputs:

$f \propto$ probability density function for node pair selection
 $F \propto$ cumulative density function for node pair selection
 Q : normalisation constant for f

```
1: function COMPUTESELECTIONPROBABILITIES( $r[], N_1, N_2, P_1, P_2$ )
2:    $f \leftarrow$  array of length  $N_1 \times N_2$ ,
3:    $F \leftarrow$  array of length  $N_1 \times N_2 + 1$ 
4:    $F[1] \leftarrow 0$ 
5:    $k, Q \leftarrow 0$ 
6:   for  $i \leftarrow 1$  to  $N_1$  do
7:     for  $j \leftarrow 1$  to  $N_2$  do
8:        $k \leftarrow k + 1$ 
9:        $p \leftarrow 1/R_{n_i, P_1} \times 1/R_{n_j, P_2}$  ▷ Weight probability of node pair being selected using (20)
10:       $f[k] = p$ 
11:       $Q \leftarrow Q + p$ 
12:       $F[k] \leftarrow Q$ 
13:    end for
14:  end for
15:  return  $f, F, Q$ 
16: end function
```

Algorithm 7 Node population swapping

Inputs:

$f \propto$ probability density function for node pair selection
 $F \propto$ cumulative density function for node pair selection
 Q : normalisation constant for f
 P_1, P_2 : sets of indices of nodes in the respective population

Outputs:

$\tilde{P}_1, \tilde{P}_2$: population sets following node population swap
 $\mathcal{A}_p$: network sortedness of network with node populations swapped
 k : index of node pair swapped

```
1: function NODESWAP( $f, F, Q, N_1, N_2, P_1, P_2$ )  
2:    $u \leftarrow U(0, 1)$  ▷ Sample from unit uniform distribution  
3:    $k \leftarrow 1$   
4:   while  $u < F(k)/Q$  do  
5:      $k \leftarrow k + 1$   
6:   end while  
7:    $i, j \leftarrow k/N_2, (k - 1) \bmod N_2 + 1$  ▷ Indices of selected population nodes  
8:    $\tilde{P}_1, \tilde{P}_2 \leftarrow P_1, P_2$  ▷ Create copies of  $P_1$  and  $P_2$   
9:    $\tilde{P}_1(i), \tilde{P}_2(j) \leftarrow P_2(j), P_1(i)$  ▷ Trial node population swap  
10:   $\mathcal{A}_p \leftarrow$  network sortedness value (17) using  $\tilde{P}_1$  and  $\tilde{P}_2$   
11:  return  $\tilde{P}_1, \tilde{P}_2, \mathcal{A}_p, k$   
12: end function
```

S3 EVALUATION OF COLLECTIVE DYNAMICS

29 For each node, the number of peaks was identified by searching for maxima with a peak prominence of
30 $0.02 \mu M$ in the Ca^{2+} timecourse (SRK) or 2 a.u. in the v timecourse (FHN) across the simulation duration.

31 For a network with N nodes, the time-dependent Kuramoto order parameter is a complex-valued scalar
32 defined as

$$z(t) = R(t)e^{i\Theta(t)} = \frac{1}{N} \sum_{j=1}^N e^{i\theta_j(t)}, \quad (S2)$$

33 where $\theta_j(t)$ is the phase of the j th node, as extracted via a mean-subtracted Hilbert transform of the Ca^{2+}
34 signal (SRK) or v signal (FHN) for node j . The argument of z , Θ , is the mean phase of the network
35 whilst its magnitude, R , measures the degree of synchrony across the network. We sample the Ca^{2+} at
36 equispaced time points $t_i = i\delta t$, $i = 0, \dots, T - 1$ and record the time-averaged degree of synchronisation:
37 $\bar{R} = \frac{1}{T} \sum_{i=0}^{T-1} R(t_i)$.