COMPLEX POWER SYSTEM RESEARCH GROUP

Energy-transfer dynamics of photosystems

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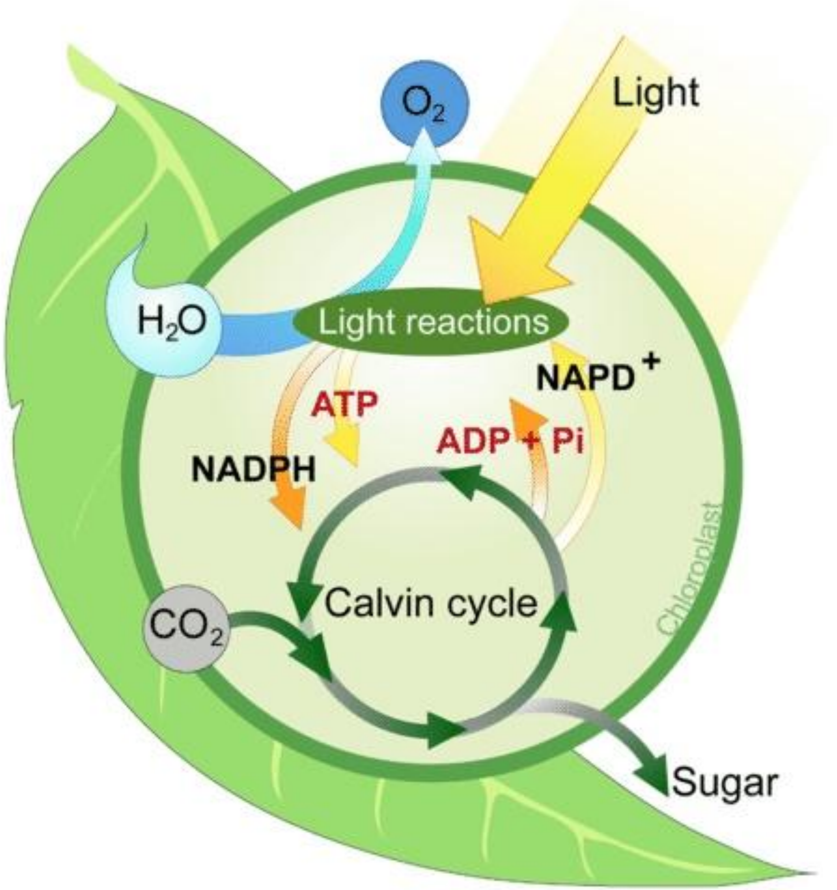
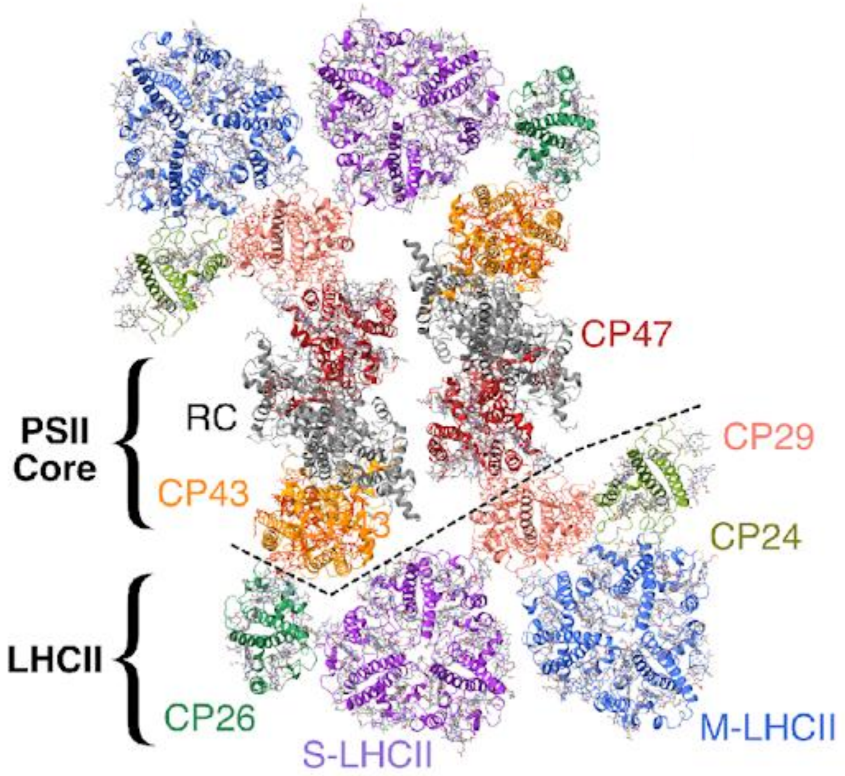
Photosystem II

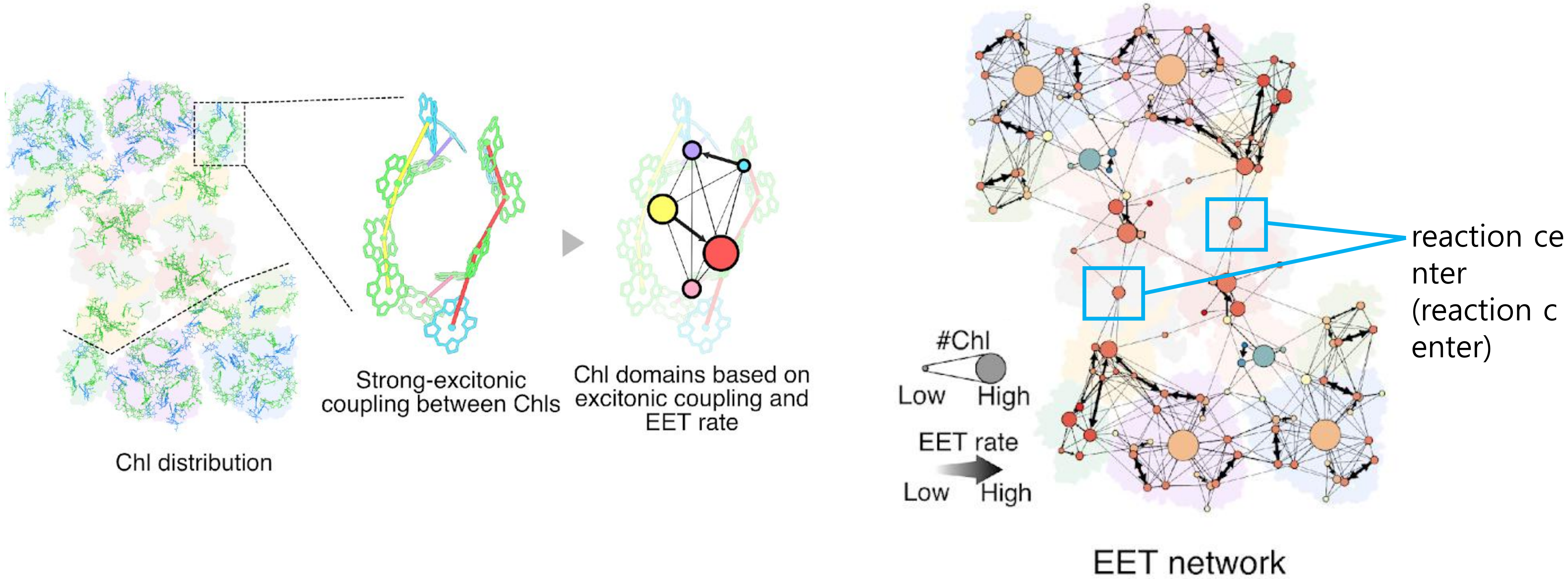




PSII–LHCII supercomplex

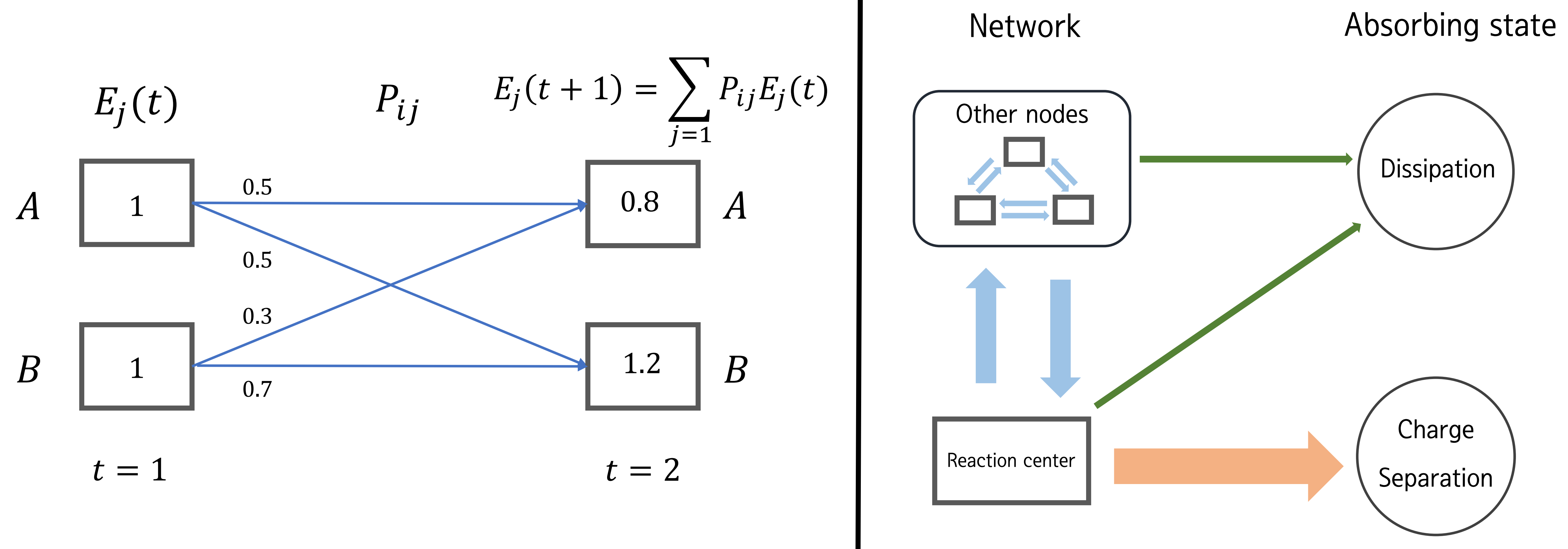
- Functional and structural unit of protein complexes that carry out photosynthesis: photosystem
- Photosystem II: A system that transfers light energy to the next process in the form of excited electrons.
- Forms a network structure of various layers through the combination of chlorophyll

Photosystem II Network



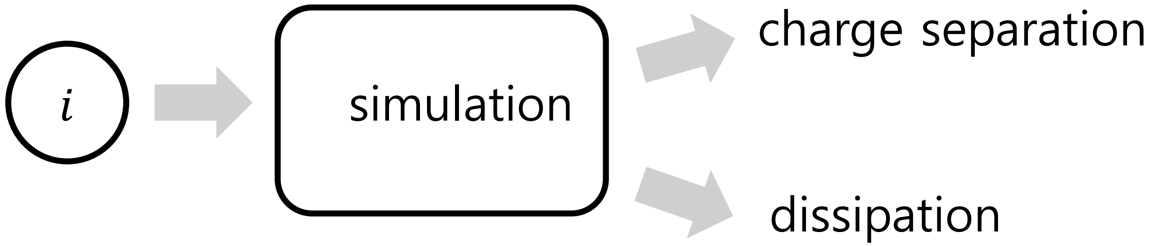
- The basic unit of a Photosystem II network: Domain
- Individual domains made up of multiple chlorophylls are defined as nodes
- The light energy absorbed by each node moves to the reaction center and is transmitted through the network structure.

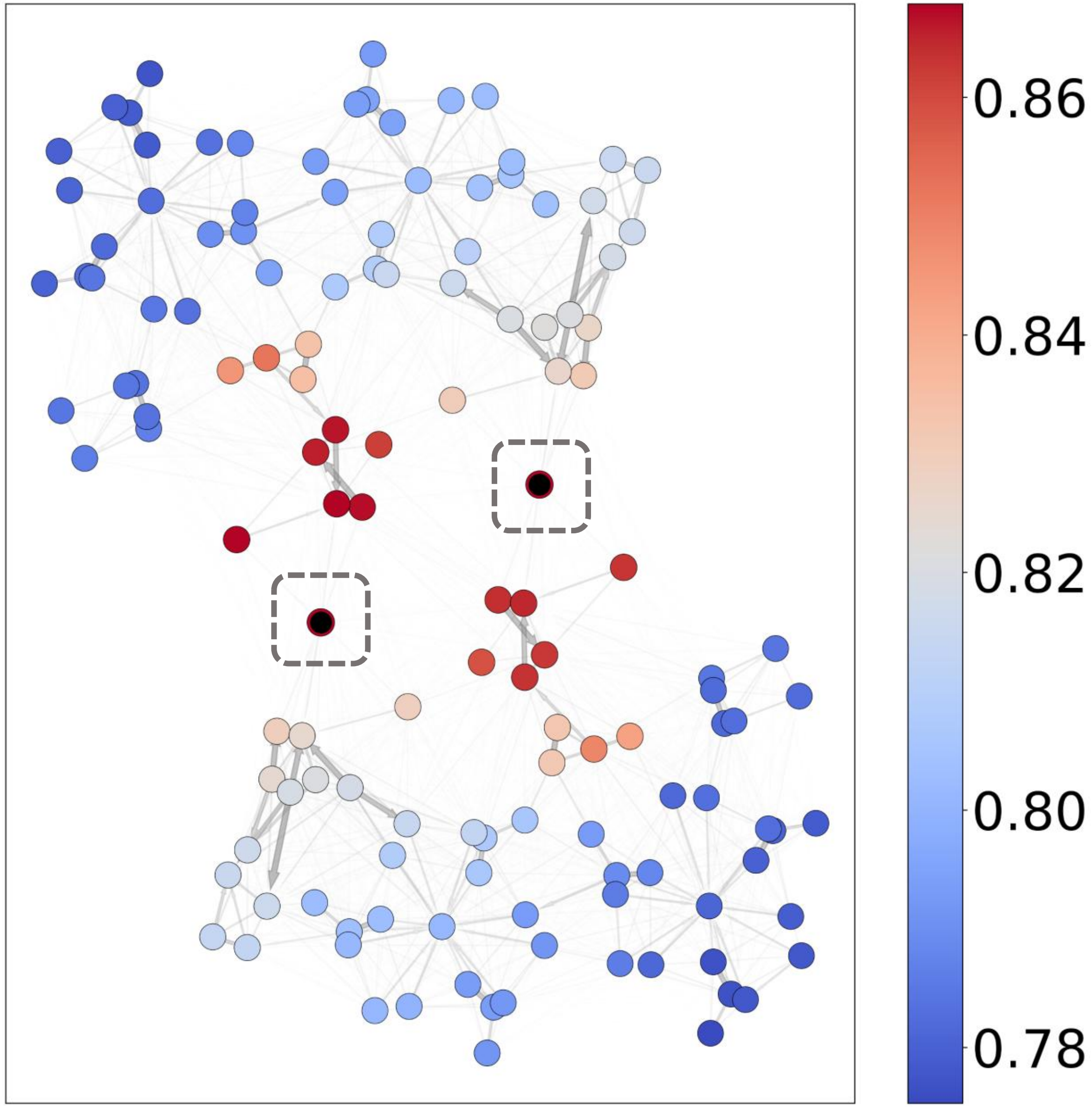
Absorbing Markov process



- Energy transfer process in photosynthetic networks: Markov process
- The energy of each node changes depending on the transition probability at every time step (0.2 ps).
- At each step, a portion of the total energy is lost, and a portion of the energy in reaction center is transferred.

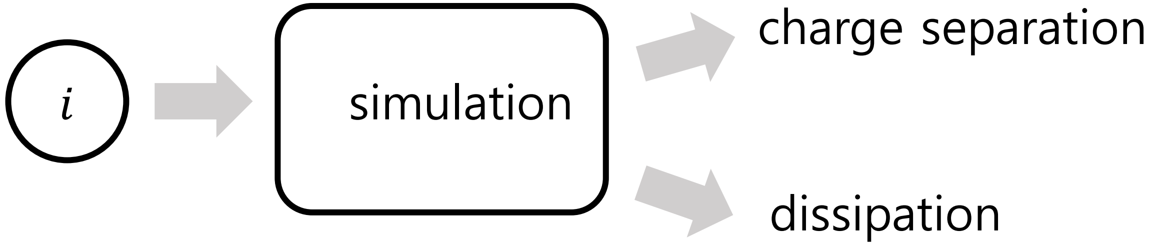
Yield of individual nodes





- Goal: analyze energy transfer in the photosynthetic network
- Inject energy into each node and measure the fraction reaching the RC
- Node color: final energy efficiency (used energy/total energy)
- Link color and direction: net transfer probability $\left(P_{ij} - P_{ji}\right)$

Yield of individual nodes



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- Inject energy into each node and measure the fraction reaching the RC
- Node color: final energy efficiency (used energy/total energy)
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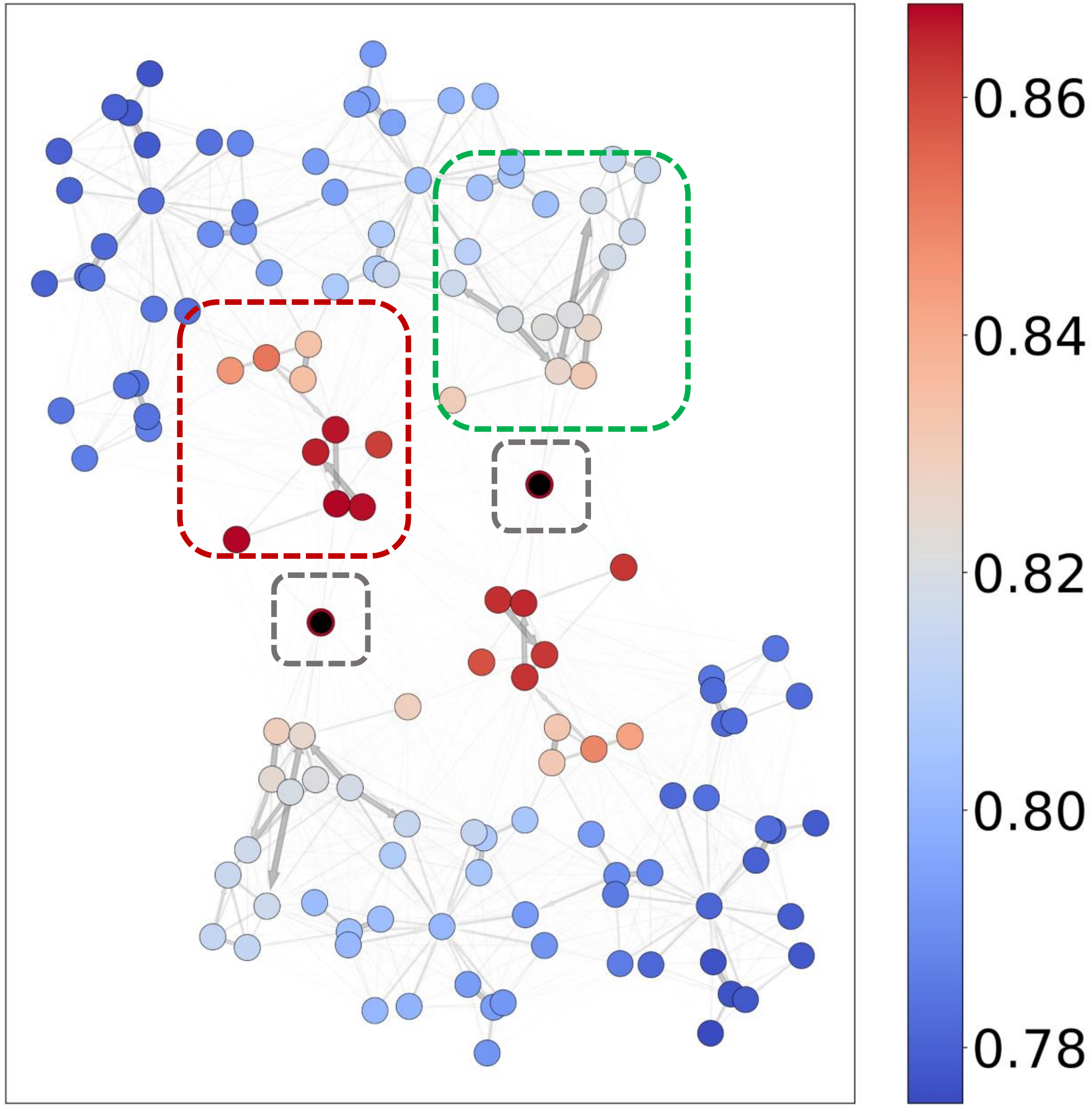
- Nodes closer to the reaction center (gray) tend to show higher efficiency.
- At similar distances, the red region shows higher efficiency
- While the green region is relatively less efficient.
- Structural asymmetry?

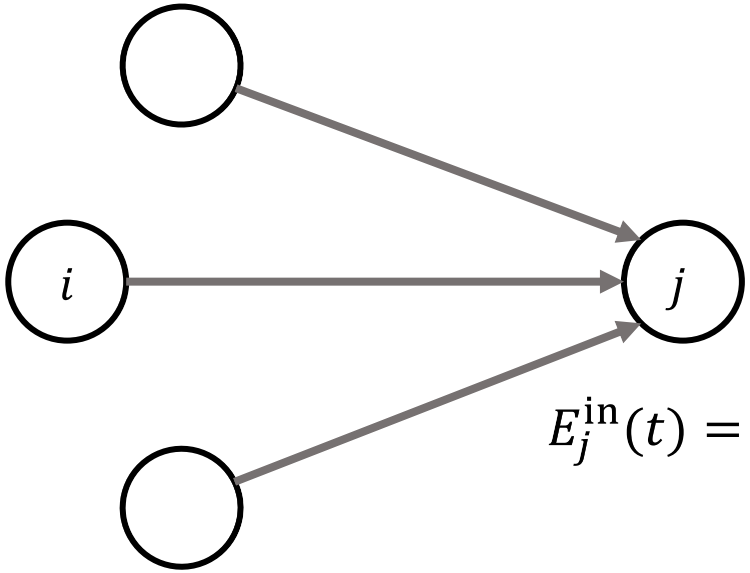


Cumulative flow analysis

- Introduce a new quantity to examine detailed energy flow.
- Track cumulative flow on each link until uniformly incident energy is fully absorbed.
- $E_i(t)$ = expected energy at node i at time t.
- Measuring link-wise energy flow and node-wise incoming energy.

$$E_i(t)P_{ij}$$

= Energy flow from i to j at time t



$$E_j^{\text{in}}(t) = \sum_{i \neq j} E_i(t)P_{ij}$$

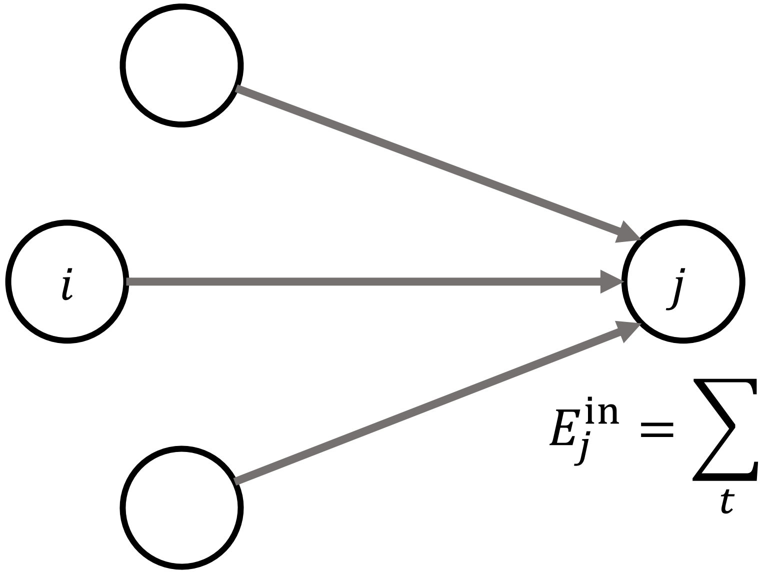
= Total energy incident on node j at time t

Cumulative flow analysis

- Introduce a new quantity to examine detailed energy flow.
- Track cumulative flow on each link until uniformly incident energy is fully absorbed.
- $E_i(t)$ = expected energy at node i at time t.
- Measuring link-wise **cumulative** energy flow and node-wise **cumulative** incoming energy.

$$F_{ij} = \sum_t E_i(t) P_{ij}$$

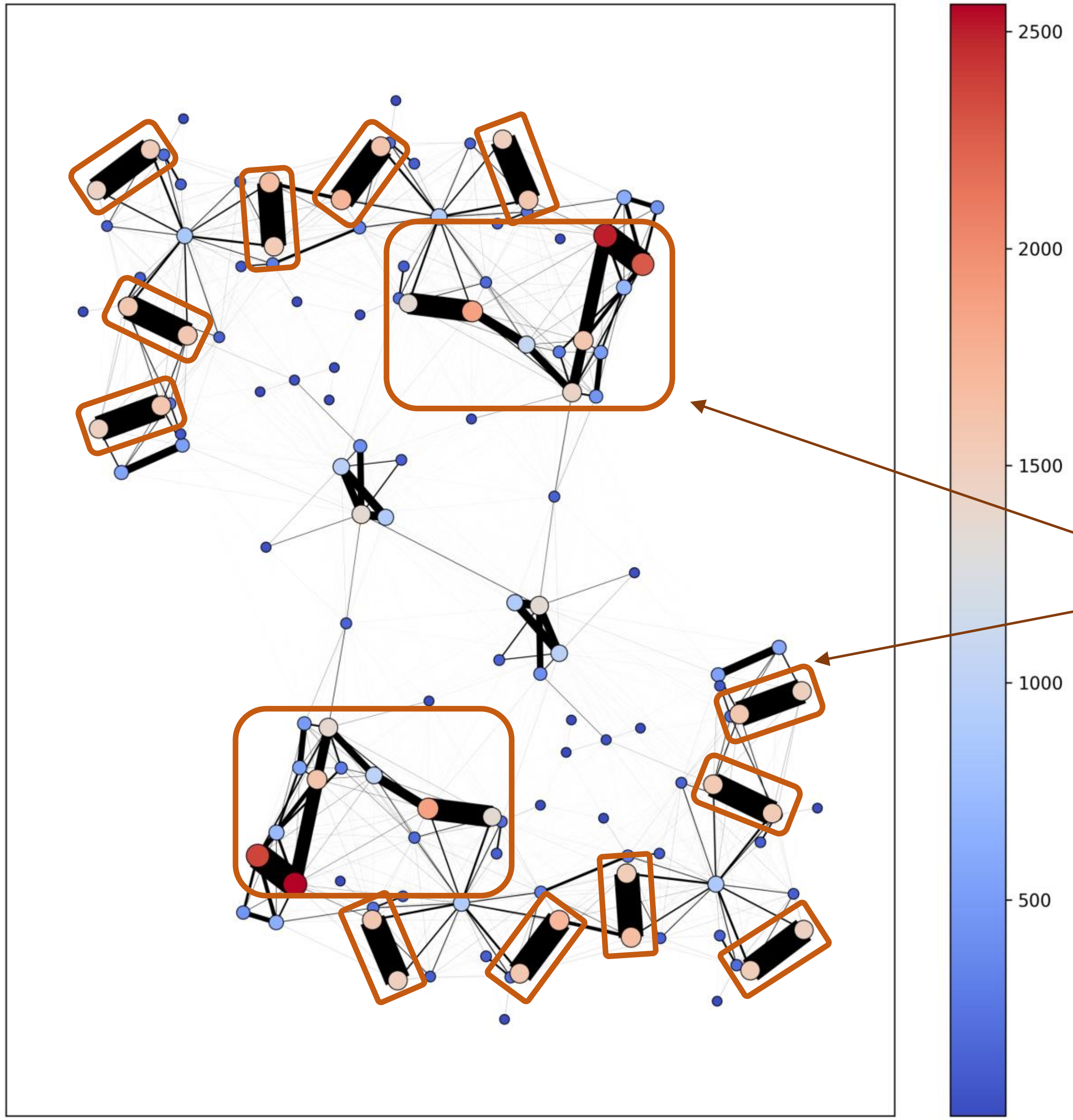
= **Cumulative** energy flow from i to j at time t



$$E_j^{\text{in}} = \sum_t \sum_{i \neq j} E_i(t) P_{ij}$$

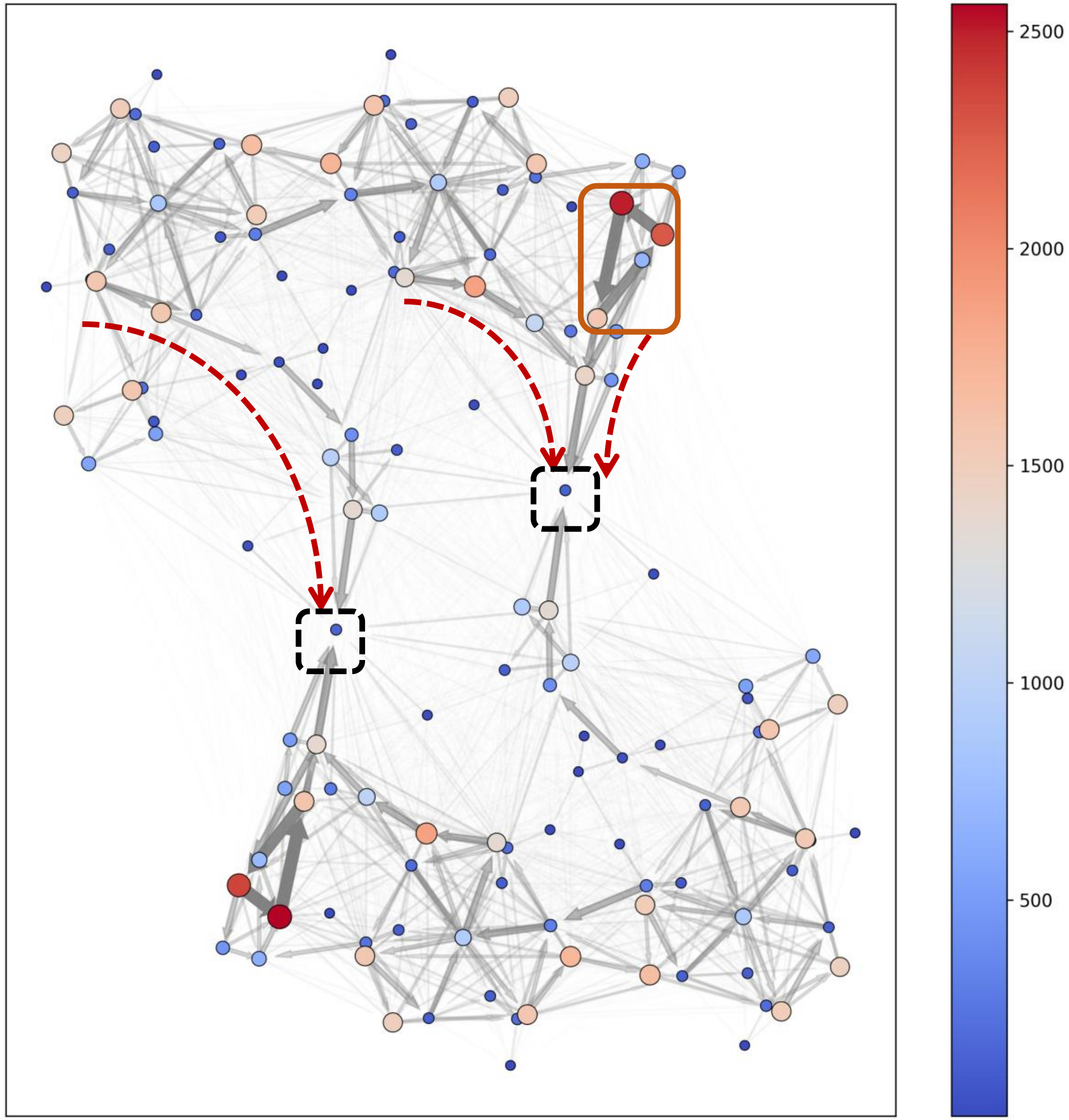
= **Cumulative** total energy incident on node j at time t

Cumulative flow analysis



- Link width: bidirectional cumulative flow $(F_{ij} + F_{ji})$
- Node color: cumulative incoming energy (E_i^{in})
- Energy flow concentrates in distinct local regions.

Cumulative flow analysis

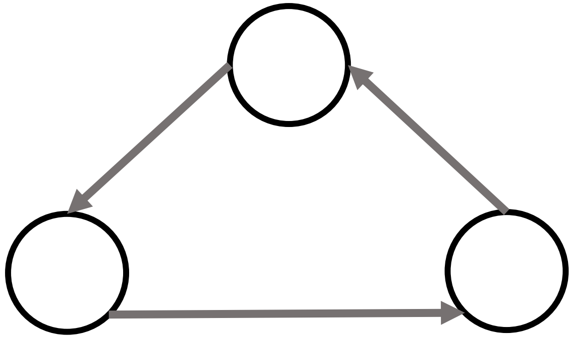


- Link width and direction: absolute difference in bidirectional cumulative flow$\left(|F_{ij} - F_{ji}|\right)$
- Loop structures appear in high-flow regions.
- Characteristic pathways that deliver energy to the reaction center emerge.

Effective loop analysis

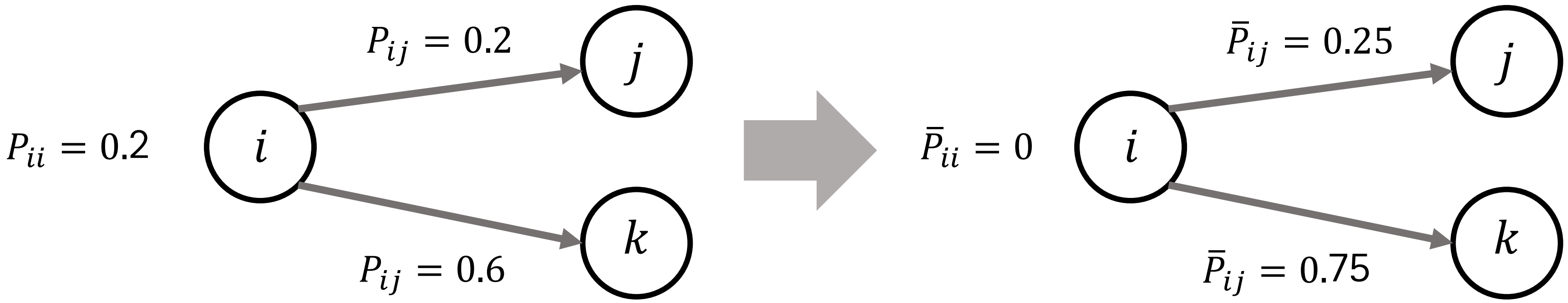
- In energy flow analysis, loop structures of various lengths exist.
- Energy originating from one node passes through another node and returns to the original node.

N=2

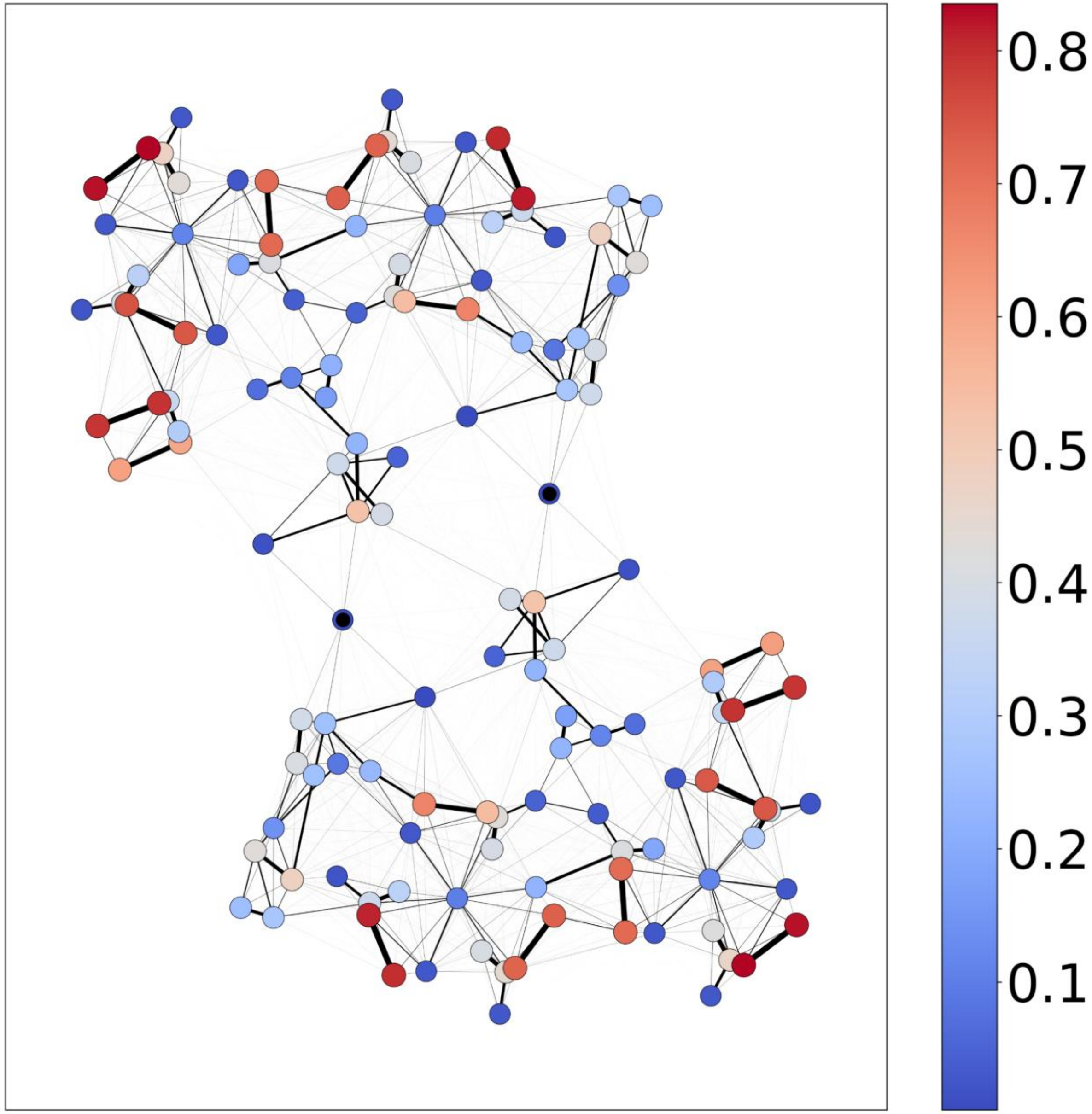


N=3

- Pure transition probability ($\bar{P}$): transition matrix that excludes dwelling probability and counts only movement to other nodes.
- Diagonal element of $\bar{P}^N$= fraction of energy returning to the original node after passing through N−1 other nodes.

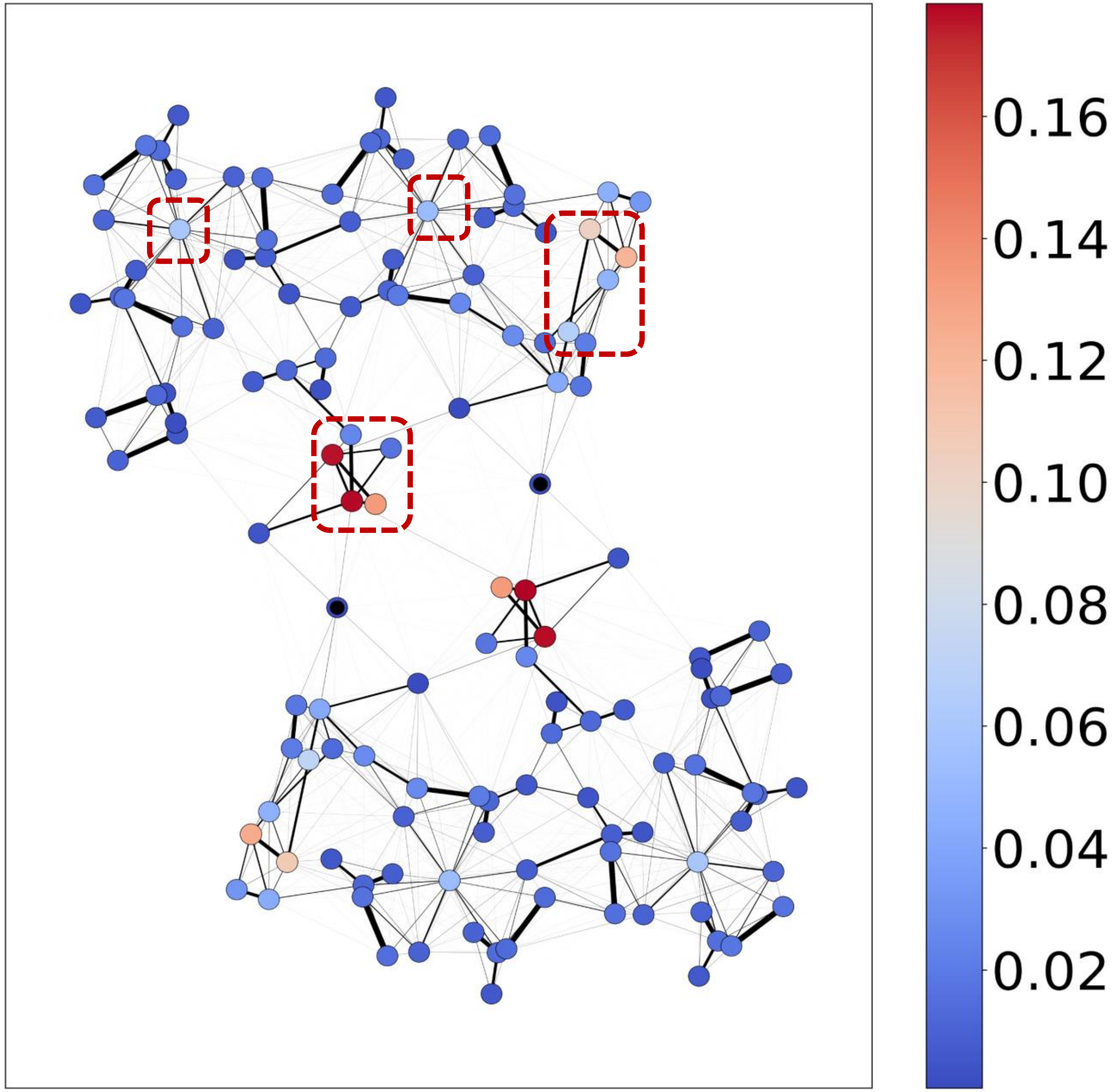


Effective loop analysis



- Link width: mean bidirectional pure transition probability $\left(\frac{\bar{P}_{ij}+\bar{P}_{ji}}{2}\right)$
- Node color: fraction of energy returning via a 2-step loop $(\bar{P}_{ii}^{2})$
- Most peripheral nodes exchange energy among themselves.
- They may act to prevent immediate absorption into the network.

Effective loop analysis



- Link width: mean bidirectional pure transition probability $\left(\frac{\bar{P}_{ij}+\bar{P}_{ji}}{2}\right)$
- Node color: fraction of energy returning via a 2-step loop $(\bar{P}_{ii}^{2})$
- Two length-3 loop structures appear in the two regions adjacent to the reaction center.

Energy-transfer dynamics of photosystems

- Analyze energy flow in photosystem network
- Perform simulation with Absorbing Markov process
- Energy efficiency analysis of individual nodes
- Discover characteristic paths through cumulative energy flow analysis
- Identify the area where energy resides through loop analysis
- Application and expansion to transportation networks, power grid networks, etc.