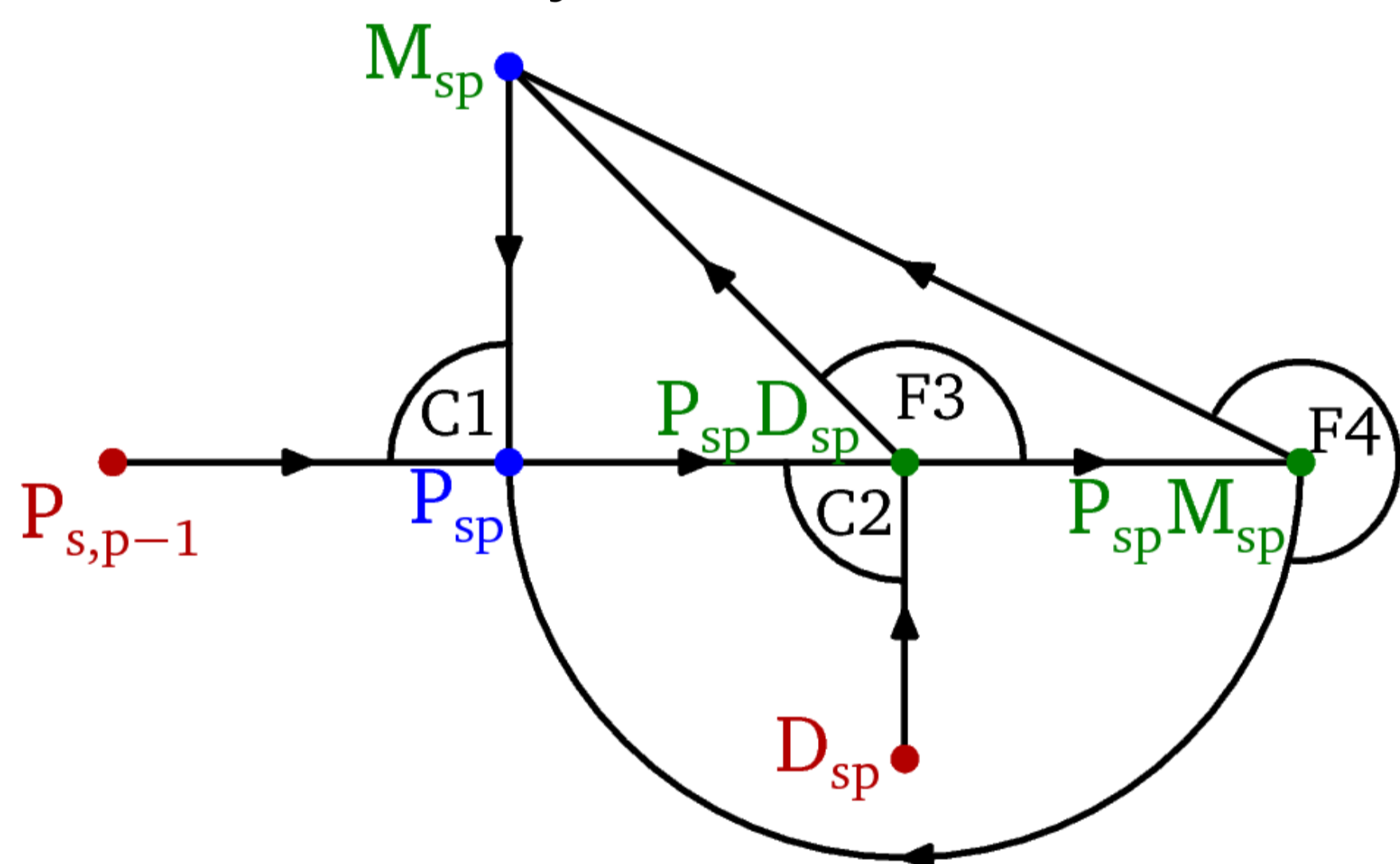


Conceptual Background Providing Inspiration for SimSoup

- Metabolic theories, including those of Aleksandr Oparin, Stuart Kauffman, Freeman Dyson, Chrisantha Fernando and Jonathan Rowe, and the Lipid World theory and GARD model of Doron Lancet's group
- Graham Cairns-Smith's clay crystal and genetic takeover theory
- Tibor Gánti's work on the principles of life and chemoton theory
- Network theory, particularly the work of Sanjay Jain and Sandeep Krishna
- The Chemical Organisation Theory of Peter Dittrich and Pietro Speroni di Fenizio
- Günter Wächtershäuser's chemo-autotrophic Iron-Sulphur World
- Linus Pauling's chemical bond theory

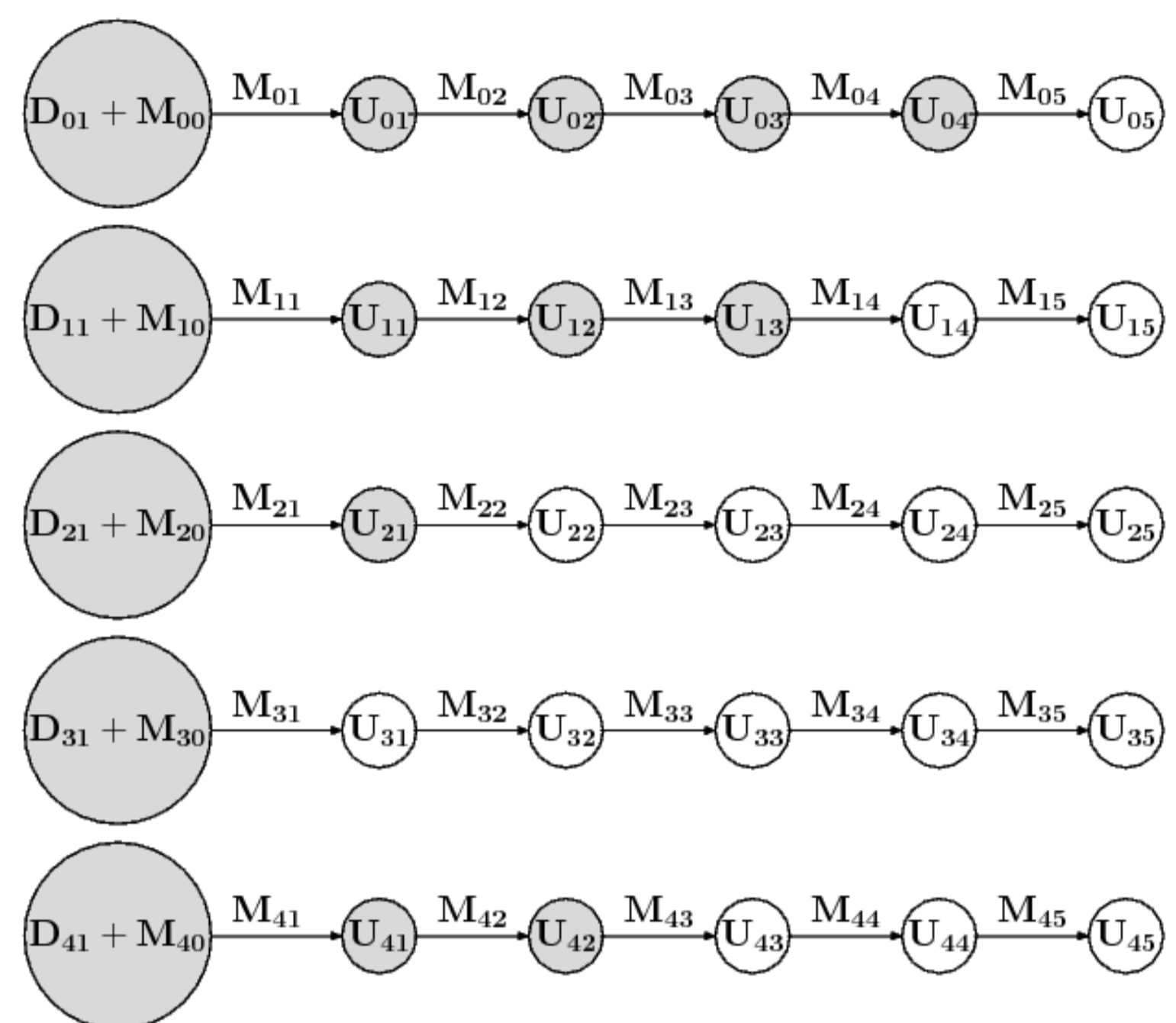
Network Structure For High Memory Capacity

Memory Unit Sub-Network



- The figure shows a two state network that forms a memory unit within a larger 'memory bank' network
- $P_{s,p-1}$ and D_{sp} are 'food'
- If a Molecule of M_{sp} is added to the food, then an Interaction of each of the four types can take place in sequence (C1, C2, F3, F4).
- Overall reaction is: $P_{s,p-1} + D_{sp} + M_{sp} \rightarrow P_{sp} + 2M_{sp}$
- The sequence can only proceed if at least one Molecule of M_{sp} is present
- Once started, the reaction maintains itself due to excess production of M_{sp}
- M_{sp} , P_{sp} , $P_{sp}D_{sp}$ and $P_{sp}M_{sp}$ are an autocatalytic set that can be activated by any member of the set

The Memory Bank Network



- The figure shows a 'memory bank' of 25 units in five independent rows or *series*
- Each unit:
 - Has a label U_{sp} , where s indicates the series, and p indicates the *position* of the unit in its series
 - Has the internal network structure of the 'Memory Unit Sub-Network'; the specific Molecule Types vary
 - May be active or inactive. Shading indicates active
 - Can only become active if its predecessor is active
- The large circles on the left represent maintained food
- In each series, the food provides the input to the first unit. The outputs provide the input to the next unit
- Each M_{sp} represents a Molecule Type that will, if introduced in very small quantities, activate unit U_{sp} , provided its predecessor is active
- Overall, the diagram represents a network in which each of the five series has 6 possible states (from no units active, to all five active)
- The network as a whole can have $6^5 = 7776$ different states. A network with ten series of nine units would have 10^{10} possible states

Molecular Structure Of Memory Units

Molecular Structure In SimSoup

Two Dimensional Rigid Structure

- Molecules are two dimensional rigid structures built from Atoms bonded together such that they occupy fixed positions on a square 'Board'
- Each square contains at most one Atom
- Bond angles are always 90° or 180°
- Bond lengths are all equal
- Atoms bond together in a way broadly consistent with valence bond theory

Atom Types Designed For Specific Purposes

- **Assemblite**: Forms two bonds. Used for structural assembly
- **Stoppite**: Forms one bond. Stops further Molecule growth at a site
- **Junctium**: Forms three bonds. Provides a 3 way junction in a structure
- **Loosium** and **Anti-Loosium**: Each forms three weak (loose) bonds. Loosium and AntiLoosium do not bond to each other
- **Grabbite**: Forms three bonds. Provides a site in a monomer for another monomer to 'grab' as part of building a polymer
- **Hookite**: Forms two bonds. Provides a 'hook' that can attach to an atom of Grabbite to form a bond as part of building a polymer
- **Perturbium**: Forms three bonds. Bonds can be perturbed by nearby Metal Atoms. This property is used in the mechanism for Dimer Splitting
- **Metal**: Forms one bond. Can perturb nearby Perturbium-Perturbium bonds, even though not bonded to Perturbium

Bonds: Joining and Splitting

- Molecules Join or Split, making new Molecule Types
- Joining must respect the 'one Atom per square' rule
- Splitting occurs by breaking the weakest set of bonds that hold the Molecule into a single unit
- Bond strengths are usually fixed according to the types of Atom at each end of a bond...
- But some bonds are perturbed (weakened or strengthened) by nearby Atoms not participating in the bond