Adding Geometry to an Artificial Chemistry

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- In our case, we model chemistry using a set of objects which each have a certain (conserved) number of bonding sites
- We allow the possibility of any two unfilled sites to bond or any two bonded sites to unbond - always binary operations
- We have also defined an algorithm for applying these bonding operations

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- Simply make the dependance setup of each light on the others random and you have an **RBN**

Why Use a Random Boolean Network?

- There is a huge space of possibilities, even for a k constant across the network we have an (overestimated) upper bound of $\left(2^{2^k} \times \frac{n!}{(n-k)!}\right)^n$ possible networks

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- So we use them as part of an AChem to produce novel, interesting behaviour in a computer

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- What is geometry like?

Description of model

- Focus on 2D chemistry
- A simple model for why things bond in real chemistry uses orbital overlap as the bonding condition
- Our model simplifies atoms to points, and orbitals to directed cone-like shapes
- The condition for bonding is simple overlap of these 'cones' (probabilistic)
- This is how we model geometric selection

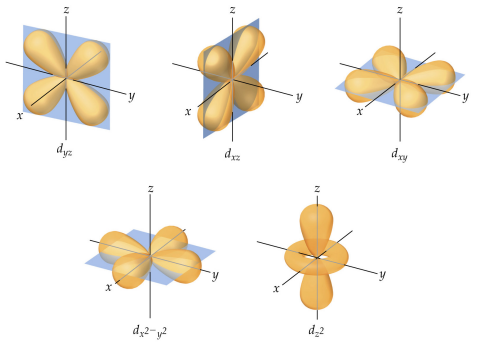

Figure : Atomic d-orbitals

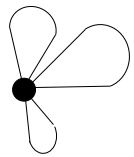

Figure : Example of possible simplified orbitals

- We still want emergent behaviour

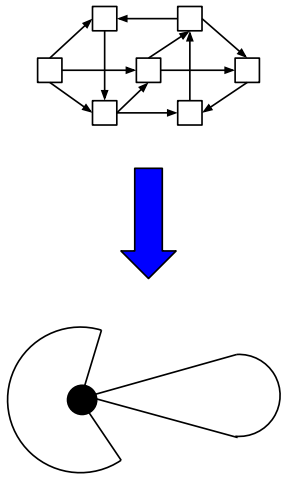

Figure : Vectors are generated from the RBN's cycle

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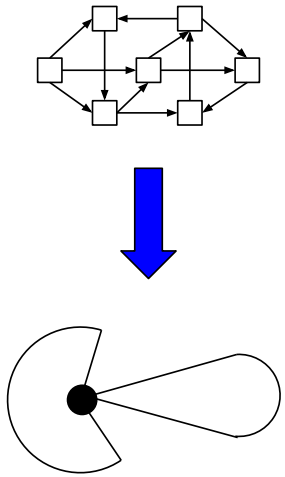

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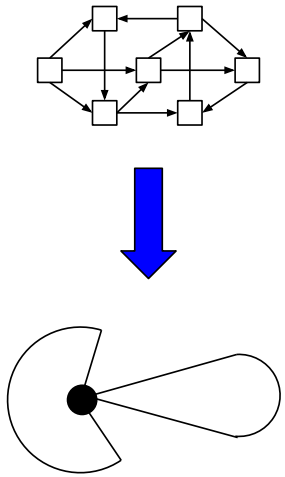
- This gives us a two-layer model where either layer can influence the other



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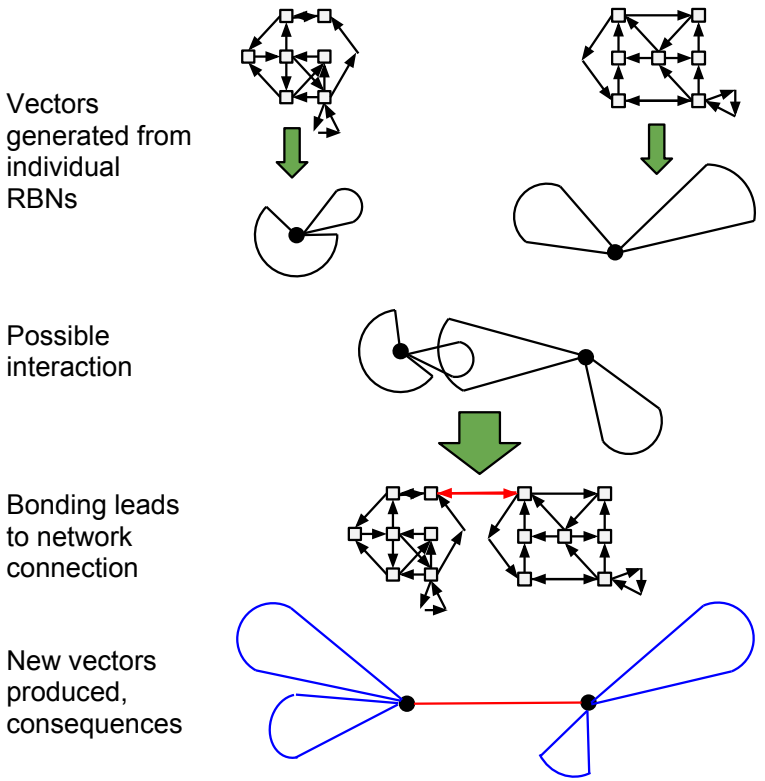

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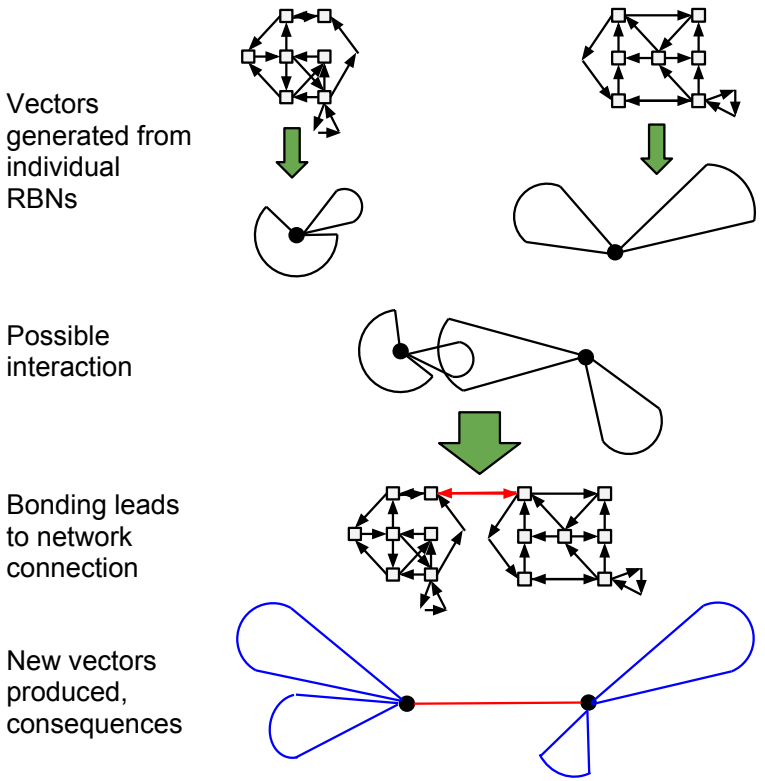

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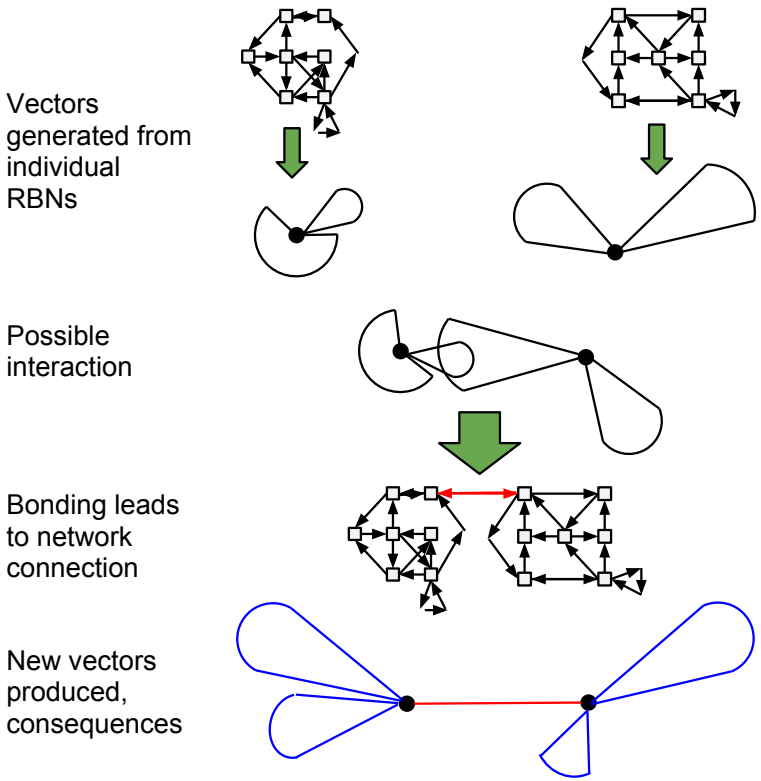

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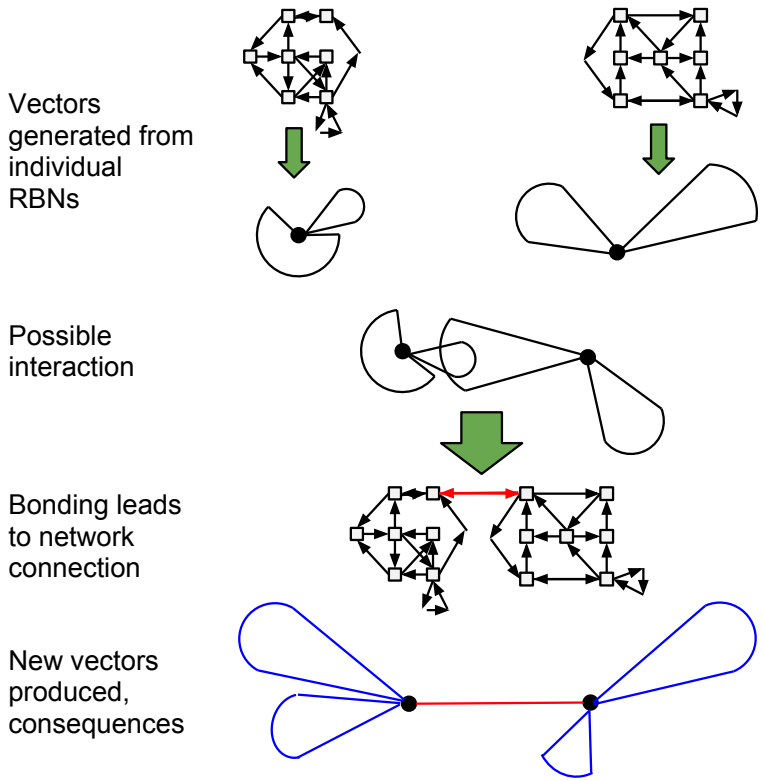

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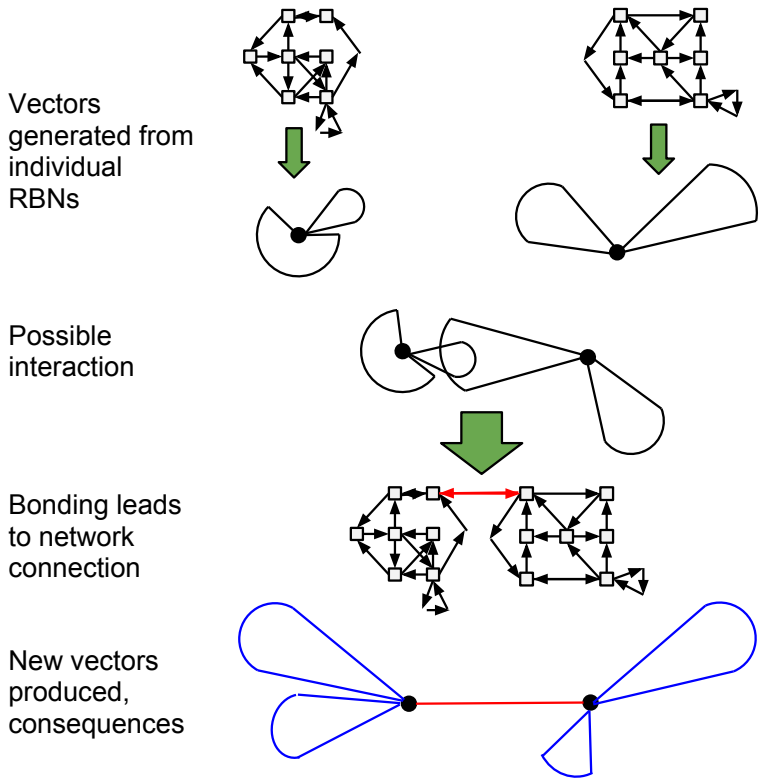
- Selectivity of certain *RBN*s for others therefore emerges naturally



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- May or may not display the rich dynamics hoped for (need more searching!)
- Difficult to see which parts model which features of chemistry
- Many arbitrary decisions involved in this feasibility study, but a smarter and more systematic search should find some interesting results!

Thank you for listening

References

http://etheses.whiterose.ac.uk/2061/1/thesis.pdf Adam Faulconbridge's thesis, involving RBNs and AChems
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