Automated Self-Assembly Programming Paradigm: Initial Investigation

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asap research
automated scheduling optimisation & planning

Outline

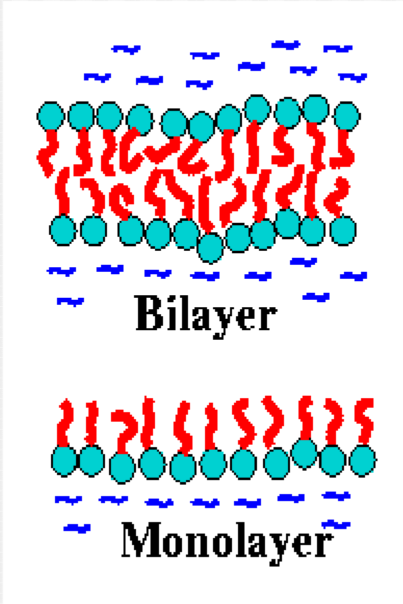
- Brief introduction on self-assembly and software self-assembly
- Automated self-assembly programming paradigm using ideal gas as a metaphor
- Experimental results and analysis
- Conclusion

What is self-assembly?

- definition:
  - Self-assembly is a process in which a disordered set of components self-organises into a specific structure.
  - Components interact with each other and form the global structure without external control.
  - The final structure is 'encoded' in the properties of components and their interactions.
- advantages:
  - Robust: replacement of failed components.
  - Versatile: prone to alternative specification.

Examples of self-assembly systems

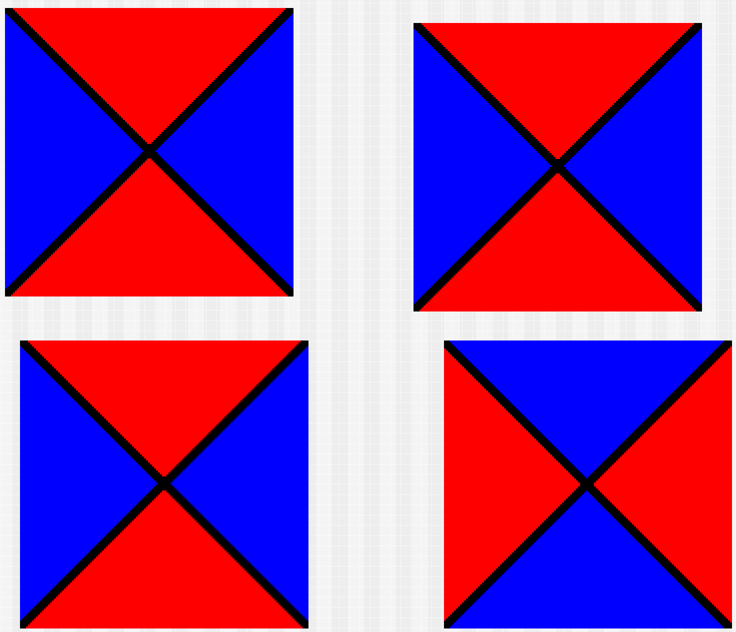
- Amphiphilic molecules
  - Formed by two ends with opposite properties:
    - Hydrophilic head: tend to be close to small water molecules
    - Hydrophobic end: tend to be close to similar chains
  - Amphiphilic molecules self-assemble into a variety of structures in water.



Examples of self-assembly systems

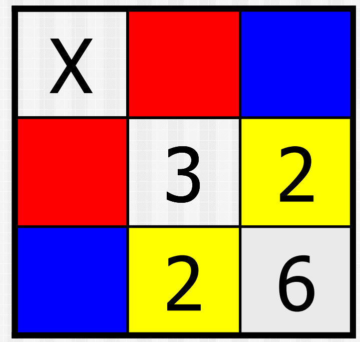
- Wang tiles model

G(blue, blue) > temp - -> tiles stick and standstill



G(blue, red) <= temp -- > tiles do not stick

Stickiness



Temp = 4

Automated Self-assembly programming paradigm (ASAP^2)

- Our automated self-assembly programming paradigm (ASAP^2) is inspired by both natural and artificial self-assembly systems.
- Software self-assembly system features:
  - human-made software components
  - software repositories
  - interaction rules
  - embodiment metaphor
  - no external intervention or central control mechanism

Software self-assembly in relation to GP

- Genetic programming: One of the most popular approaches to automated program synthesis and has been applied to wide range of problems.
- Software self-assembly seeks to provide at least a complement but maybe an ***alternative*** to genetic programming.
- GP uses natural selection as a metaphor.

This Research

- We aim at analysing the potential and limitation of software self-assembly.
- In this talk, we aim to find out how different environment settings affect an *unguided* process of software self-assembly.
- The embodiment we use is a metaphor based on ideal gas theory.

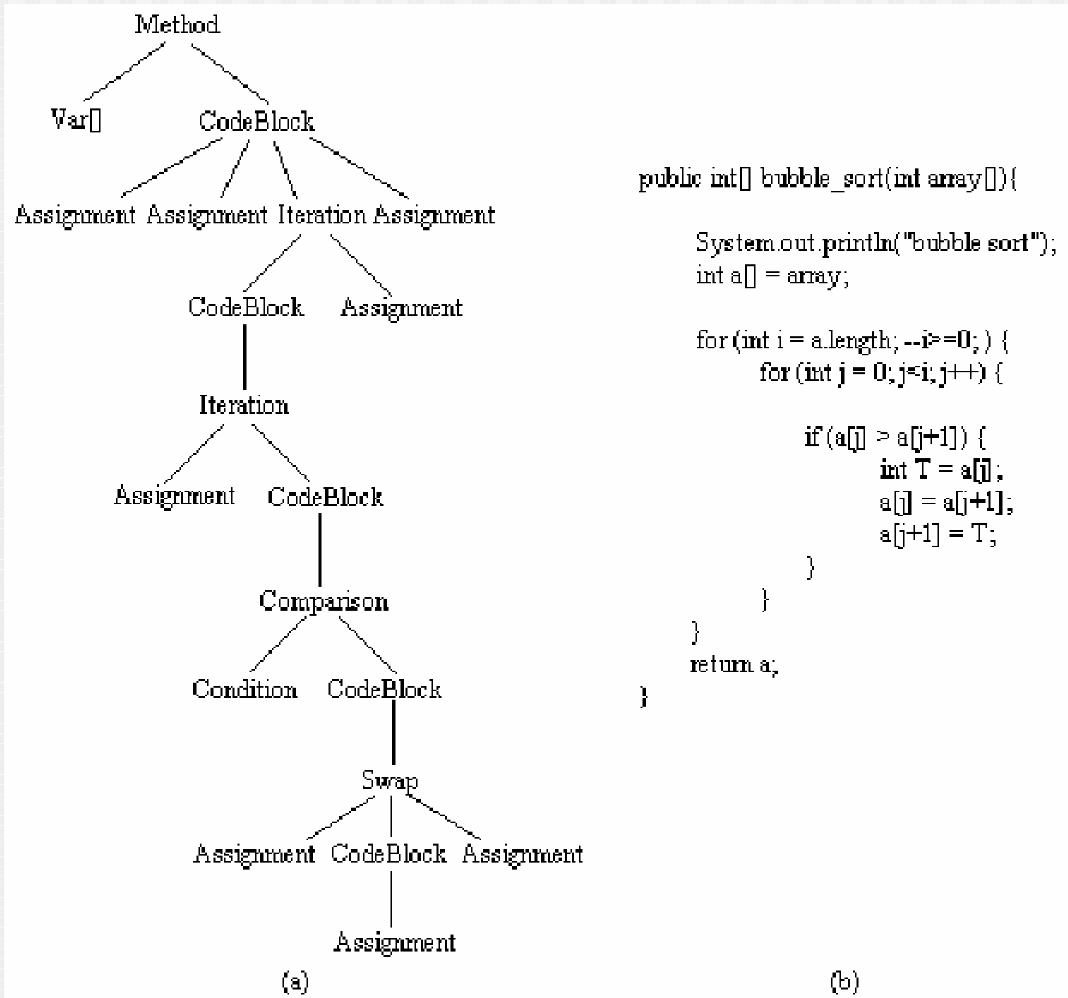
Program gases

- Our software self-assembly system is based on the theory of perfect gases.
  - Manually decomposed software components are placed into a container within which they move randomly.
  - The temperature (T), number of components placed into the pool (n), and the size of the pool (V) are free parameters of the model.
  - Components move faster as temperature increases.
- $PV = nRT$

Program gases

- What the metaphor does NOT capture:
  - Software self-assembly may bind rather than collide.
  - The size of an assembled gas component grows.
  - In perfect gases, it is assumed that the distance between molecules are much greater than their sizes.
- We investigate to what extent the equation for perfect gases holds for program gases.

A parsing tree of a bubble sort program



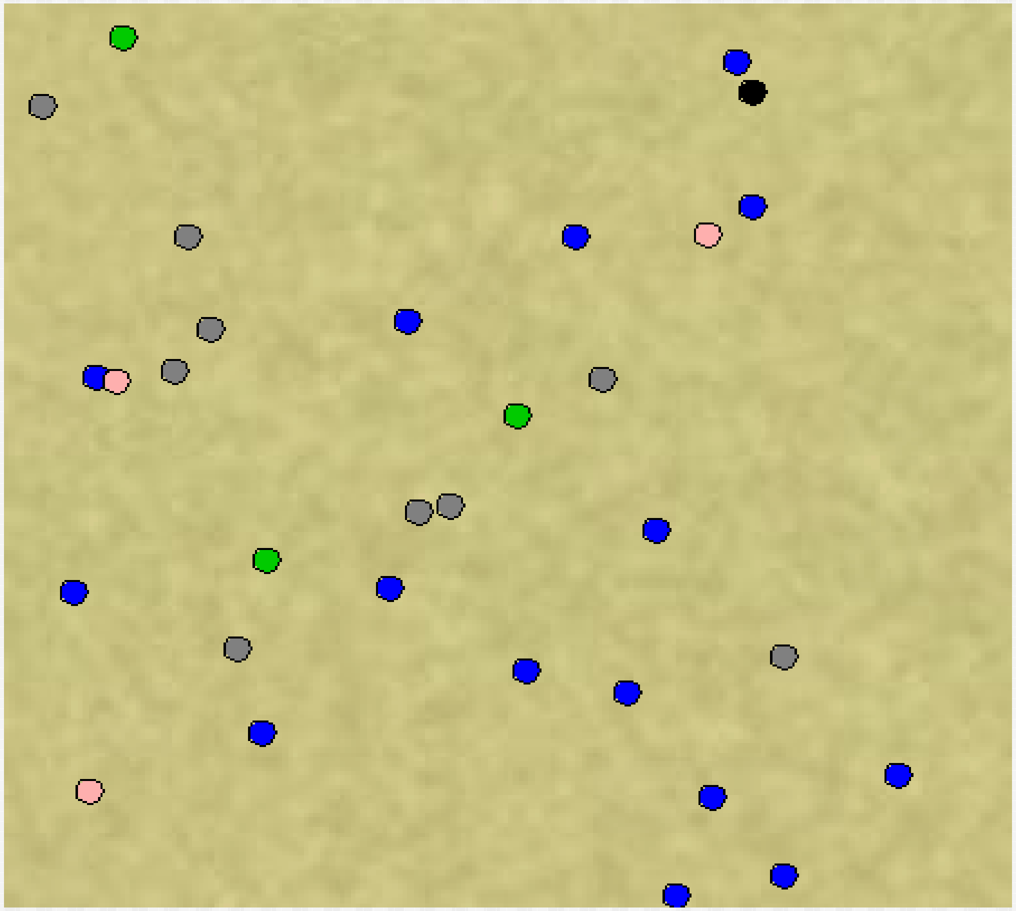
Components and ports

- Components are decomposed from a selected program and stored into a software repository.
- Each component has one input port and can have several output ports.
  - A port is used as a binding site.
  - Each port has a type associated.
- An input port can only connect with an output port of the same type.

Model descriptions

- ASAP^2 starts by placing components retrieved from the repository into the pool.
- Components move around in the pool randomly with a probability which is a function of the temperature.
- When two components are within certain proximity and their types on the connecting ports match, they self-assemble.
- Equilibrium is reached when there are **no more possible binding actions** among components left in the pool.

A gif animation of our system



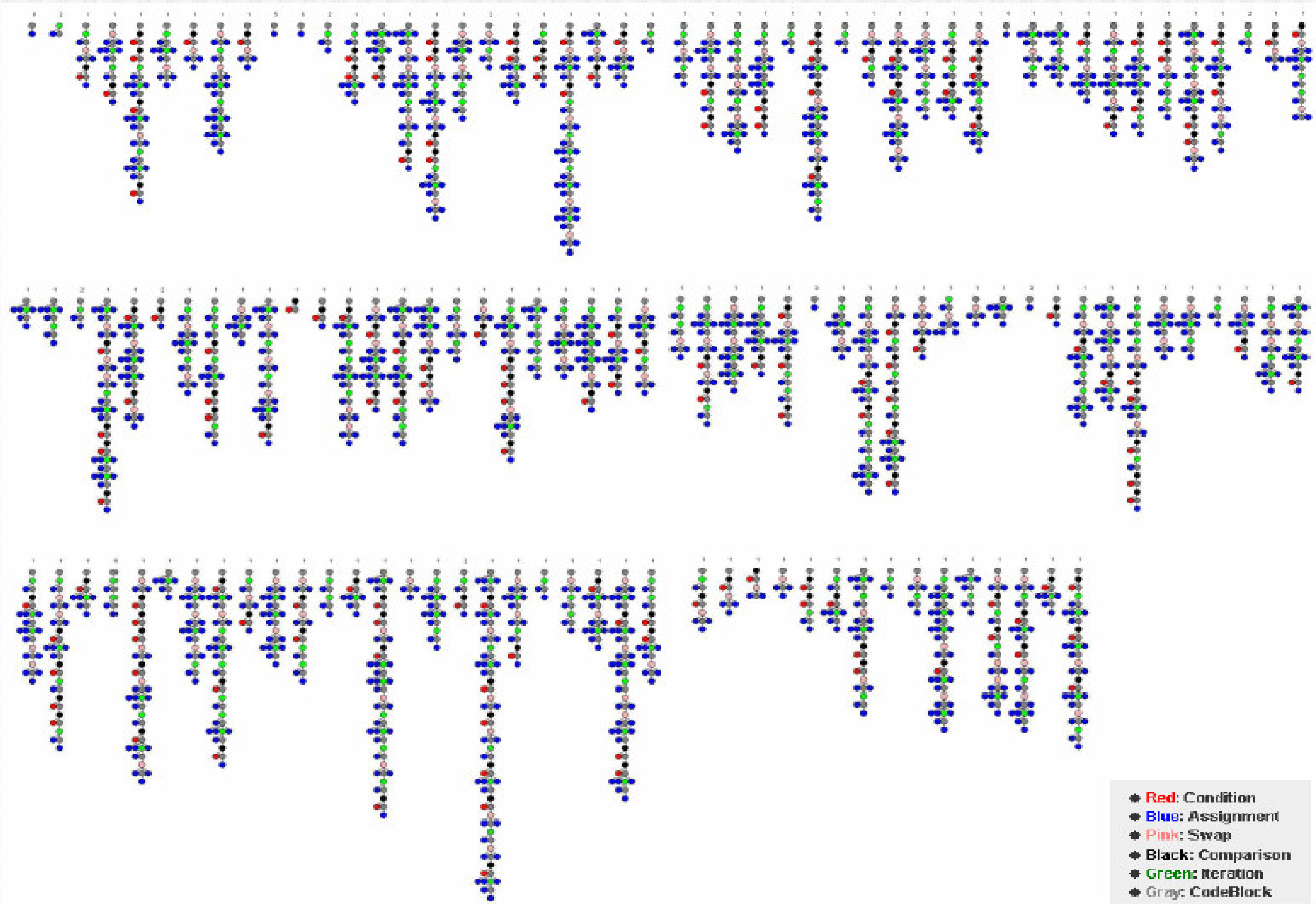
Experiment methods

- Moving probability of a component is affected by temperature: $p(M) = e^{-T}$
- Interaction distance between components is affected by the size of the component (i.e. the number of nodes in the tree).
- With three free parameters T, A and n, we measure:
  - pressure (P): number of hits on the wall
  - time to equilibrium (t_ε): time needed for the system to reach equilibrium
  - diversity of the self-assembled trees at equilibrium (D_ε): total number of different parse tree classes.

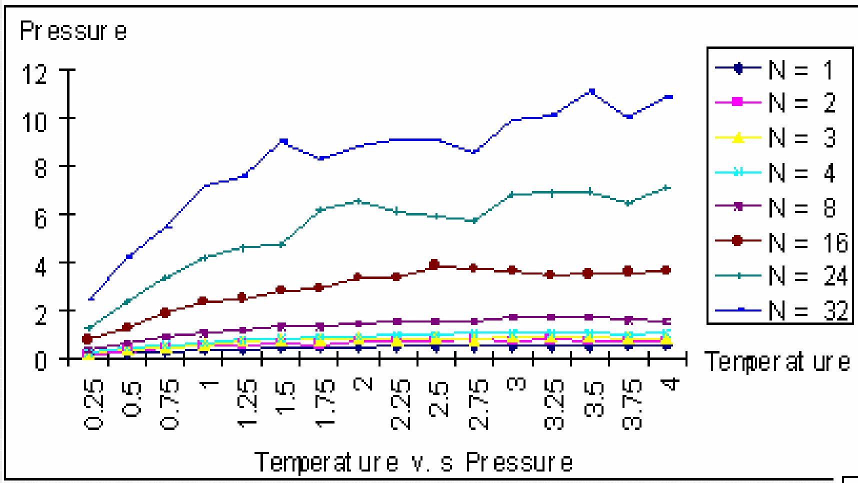
Experiment methods

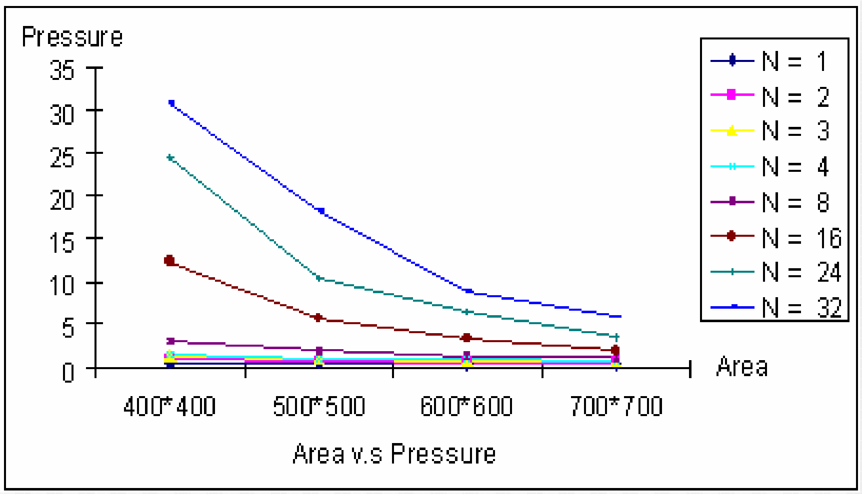
- Three standard sorting algorithms are chosen as sources of software components.
- For each of software component repository, we run 20 replicas for each (A, T, n) triplet.
- $A \in \{400, 500, 600, 700\}$, $T \in \{0.25, 0.5, \ldots, 3.75, 4.0\}$, $n \in \{1, 2, 3, 4, 8, 16, 24, 32\}$.

An example "forest" of program trees



Experiment results (bubble sort)





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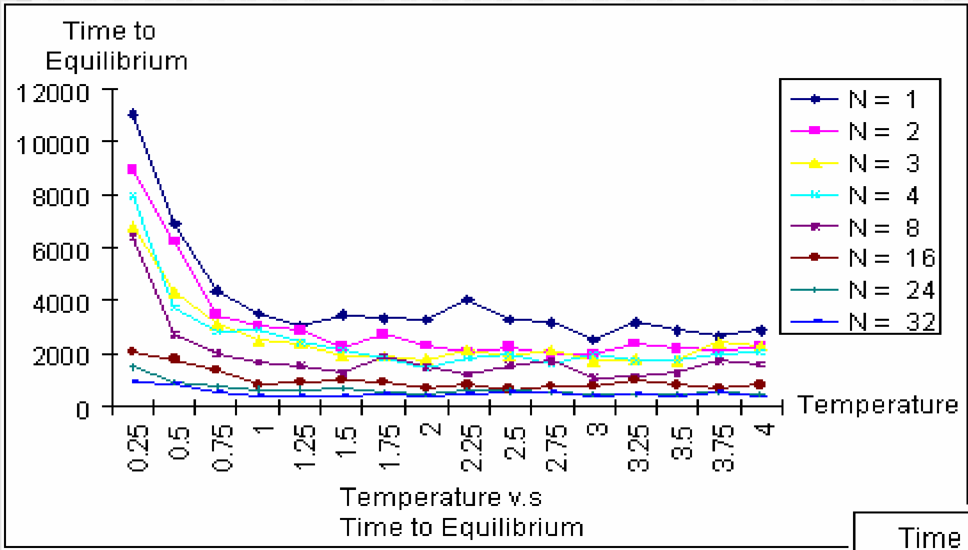
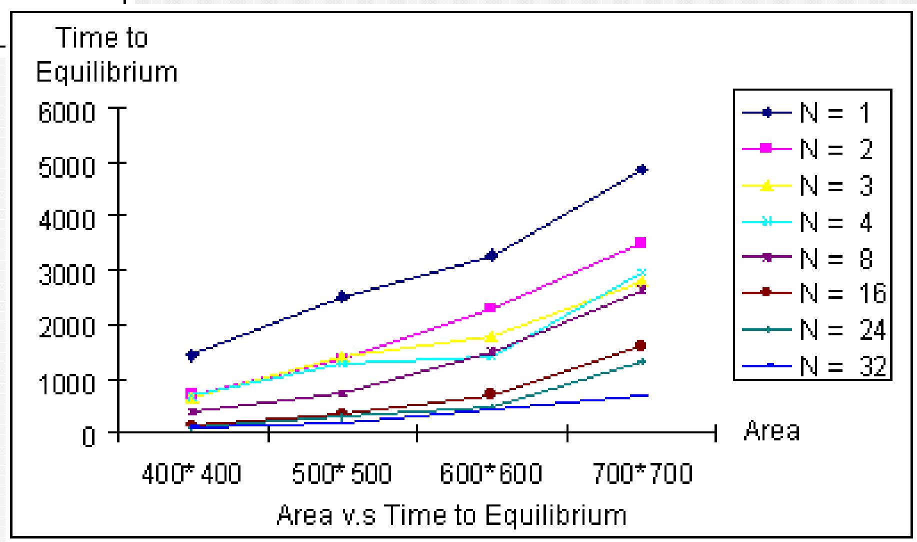
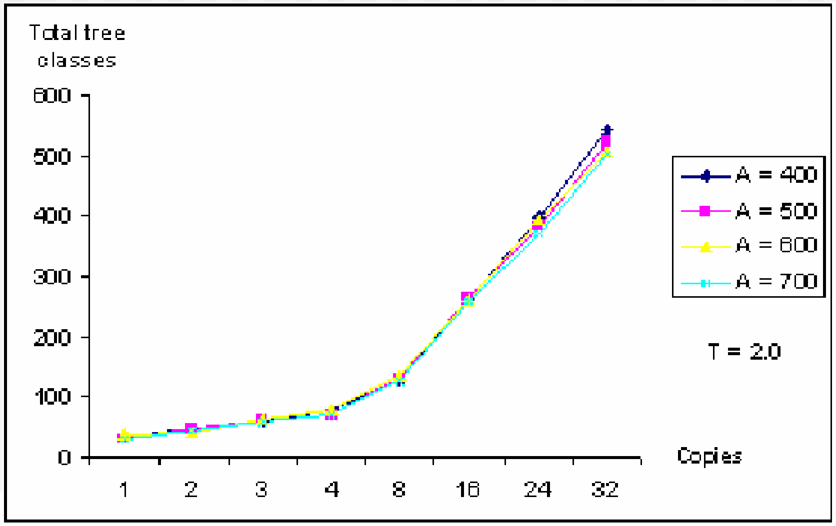
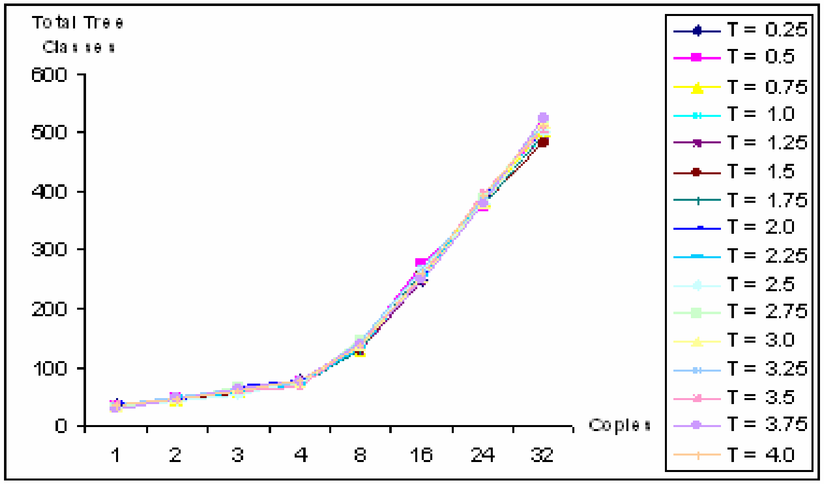


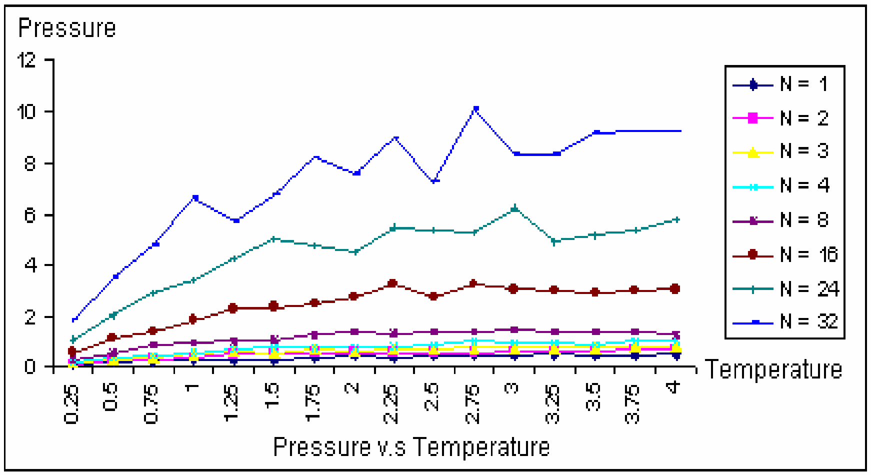


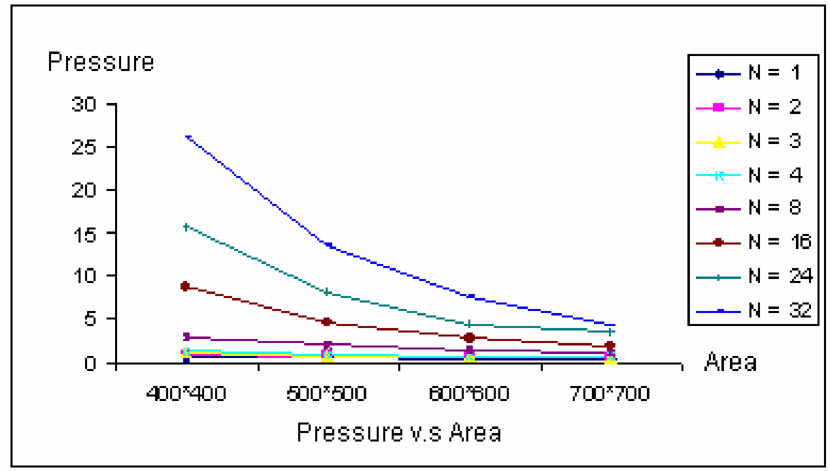
Experiment results (bubble sort)

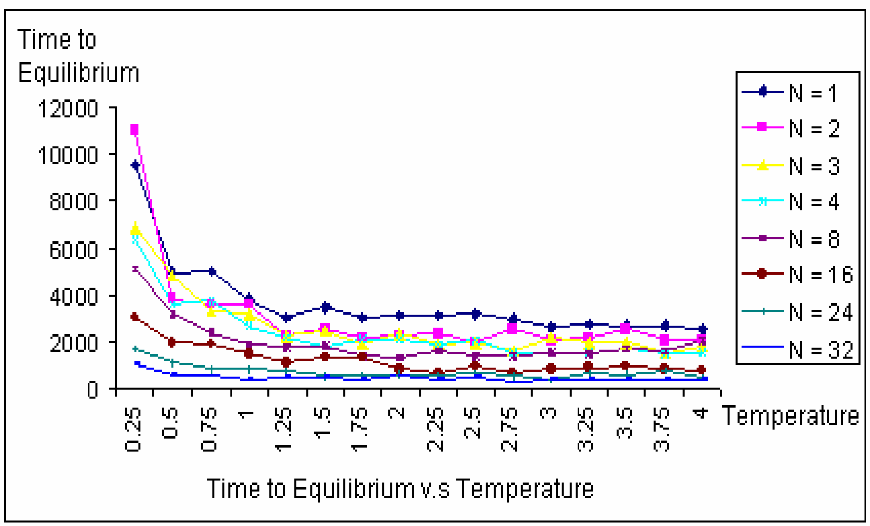


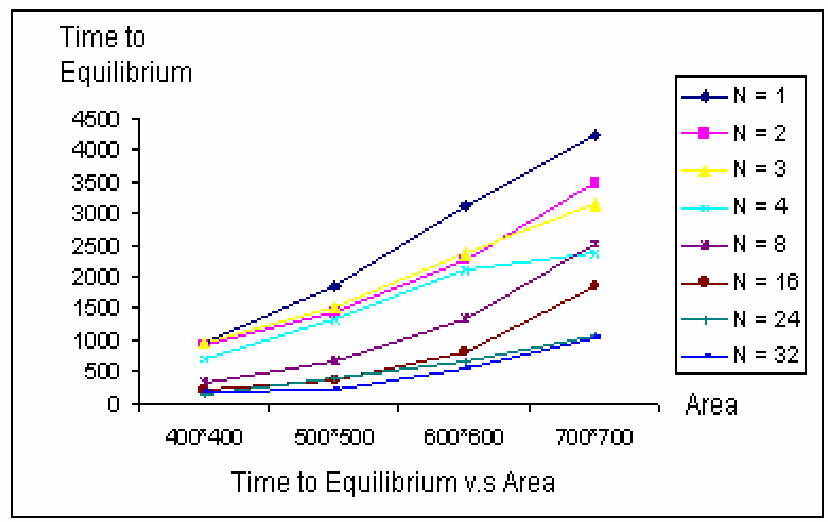


Experiment results (insertion sort)

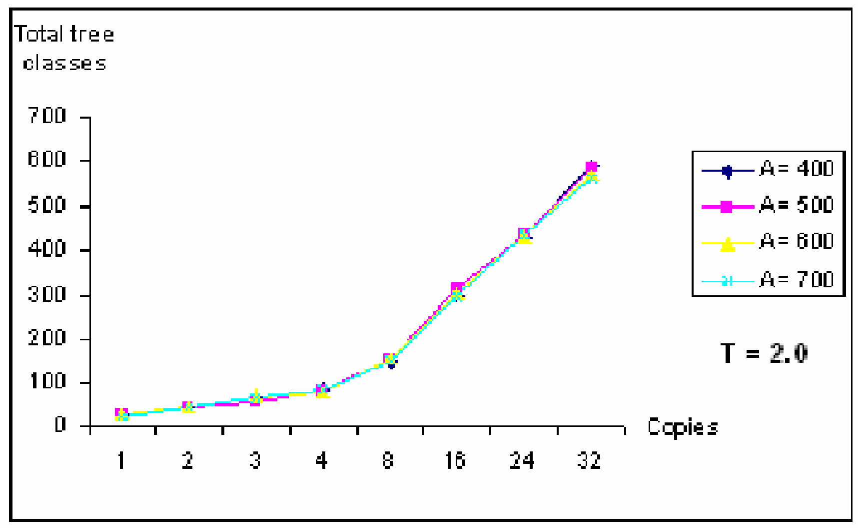


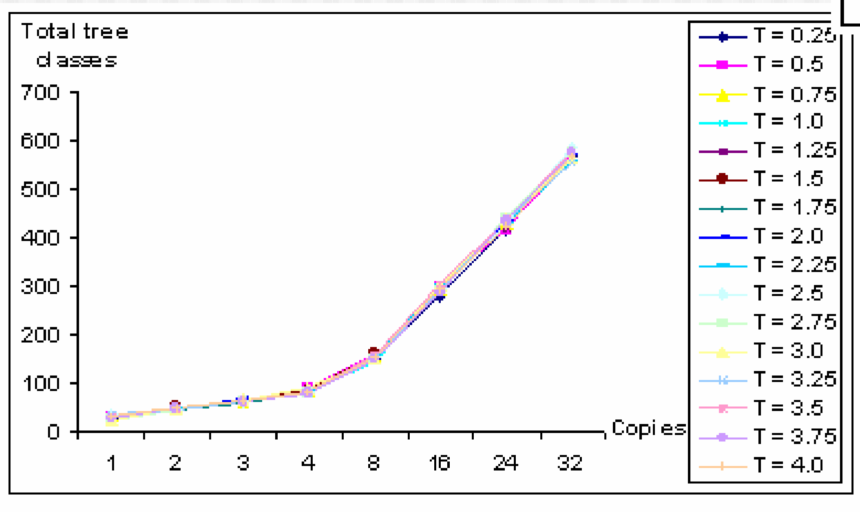




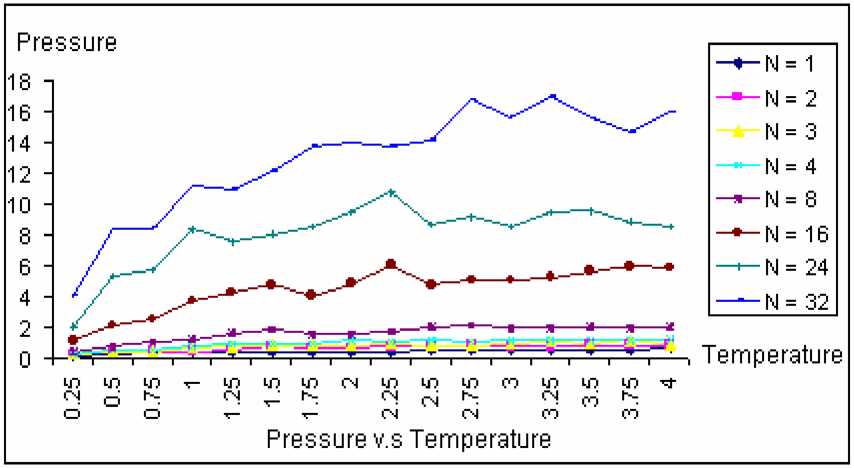


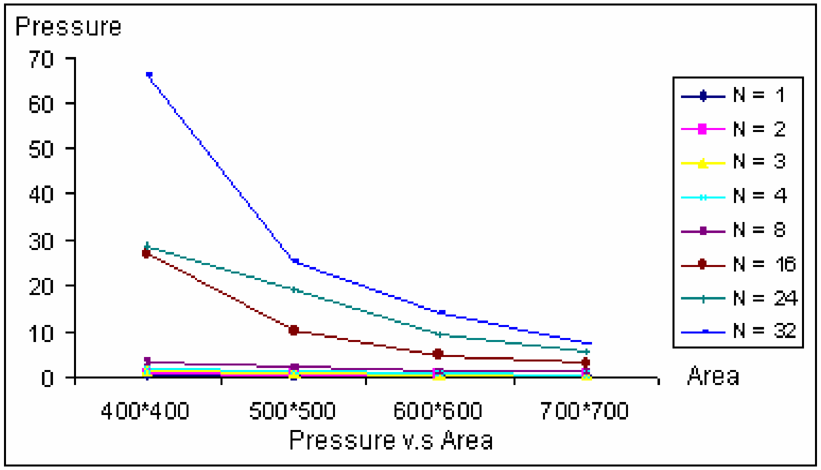
Experiment results (insertion sort)

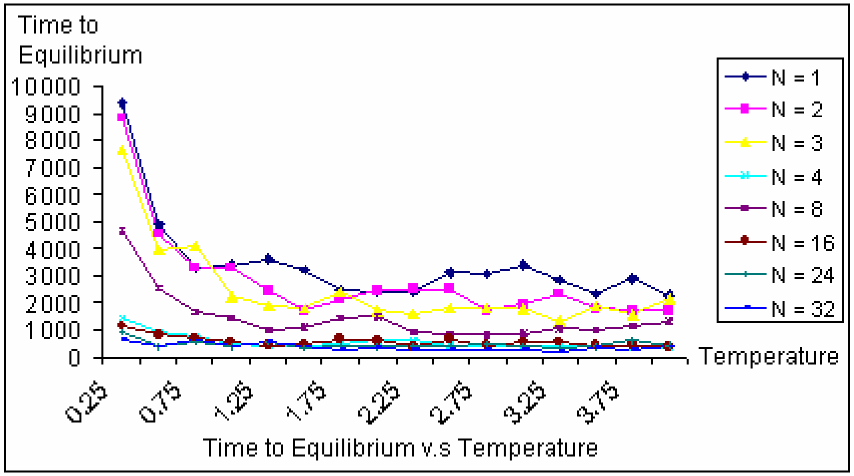


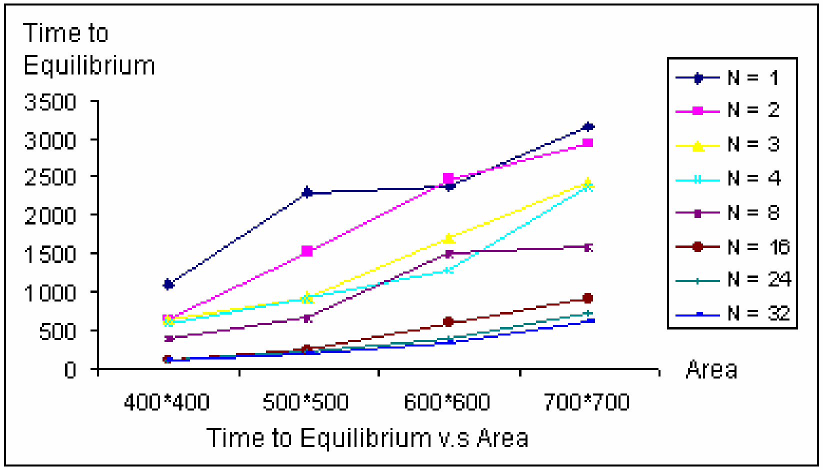


Experiment results (selection sort)









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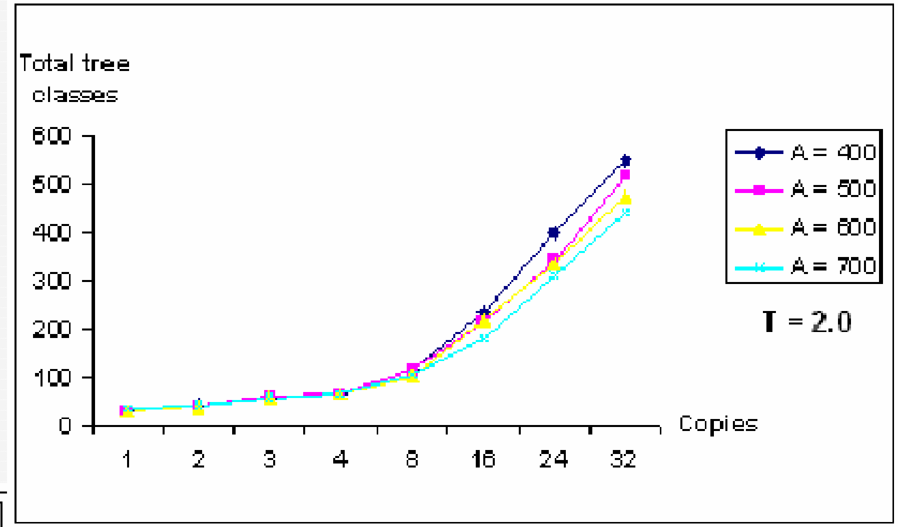
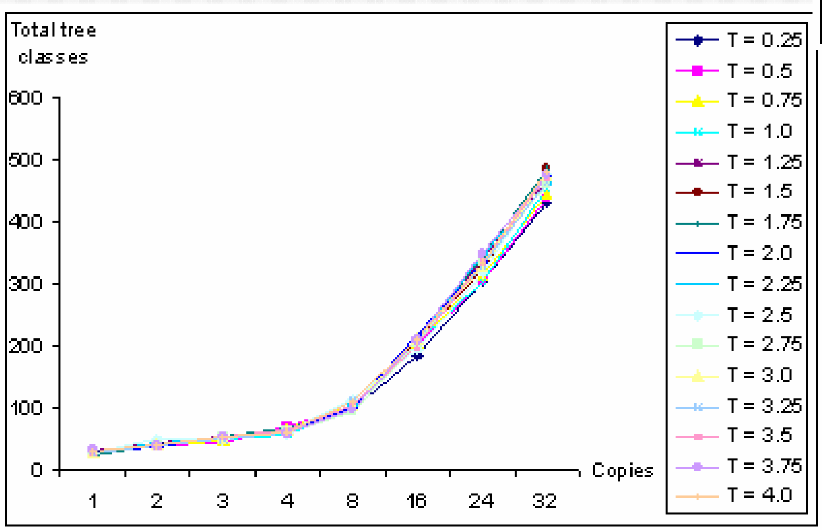


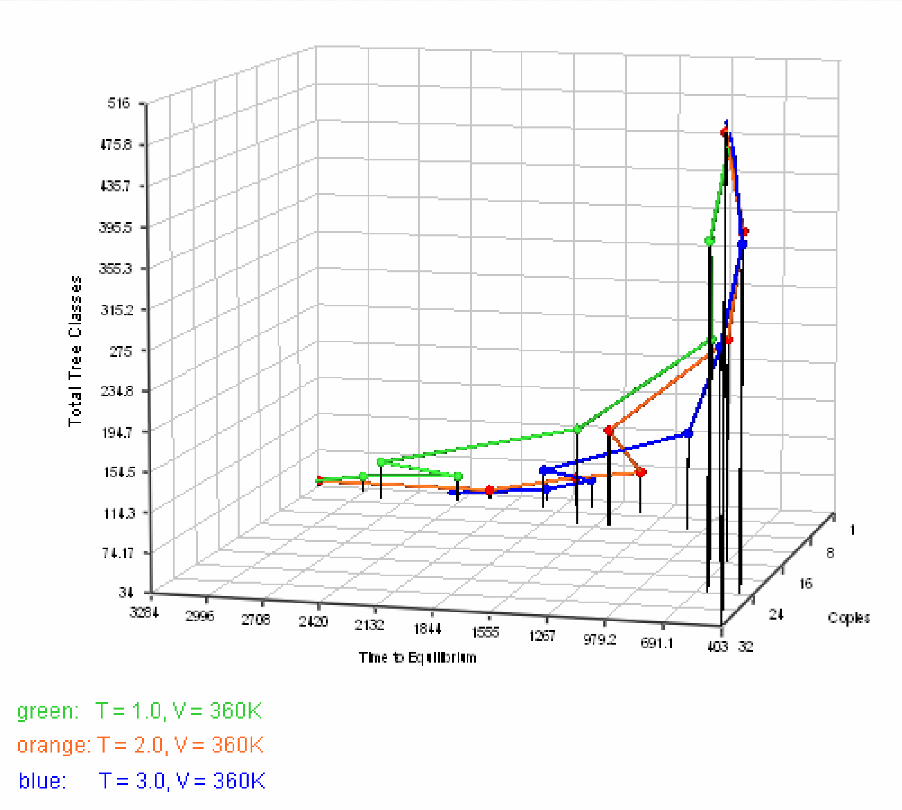


Experiment analysis

- As the equation of ideal gases suggests:
  - Pressure increases when there is a rise in temperature or number of components placed into the pool.
  - Pressure decreases when size of the pool becomes larger.
- Self-assembly can be made more efficient with:
  - Greater number of components placed into the pool.
  - Smaller size of the pool.
  - High temperature.

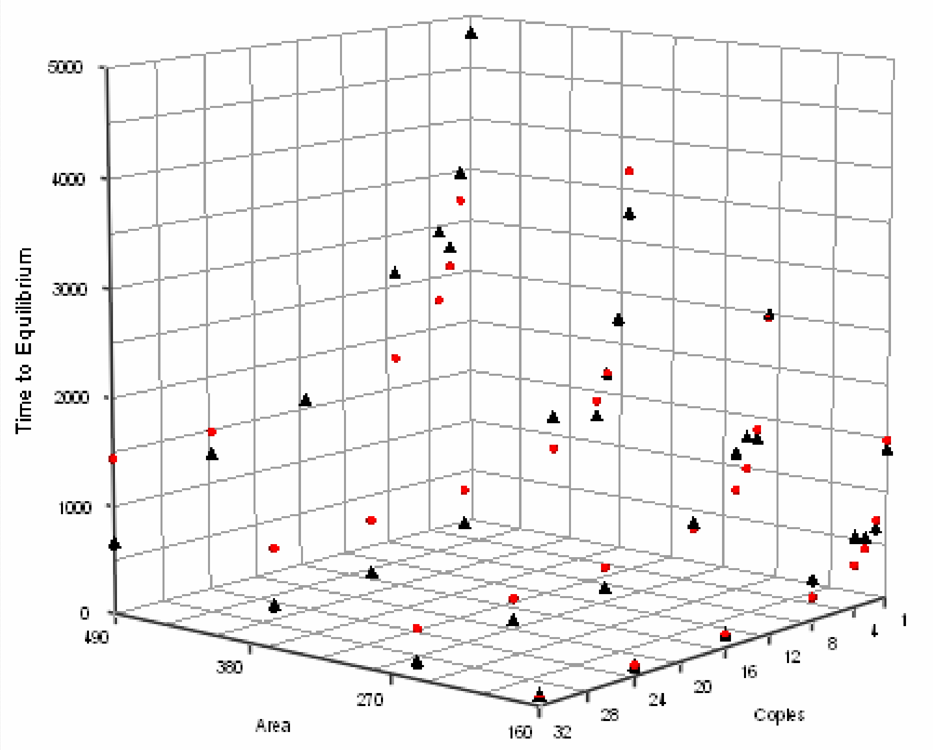
Experiment analysis

- Diversity of the generated programs are mainly affected by number of components placed into the pool.



Predictive formulae

- $t_\varepsilon(A,N) = (((7.05 * A) + 321.2) / N) +(3.91 * A) – 593.71$

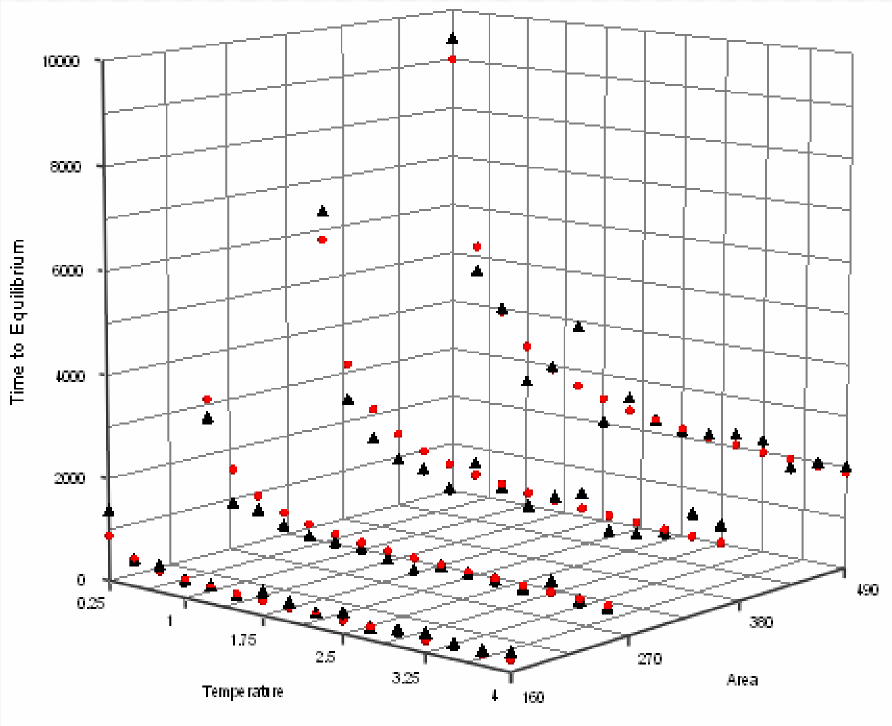


black triangles: experimental data;

red circles: corresponding data obtained using predictive model.

Predictive formulae

- $t_{\varepsilon}(A,T) = (((5.22 * A) – 659.02) / T) +(3.73 * A) – 416.11$



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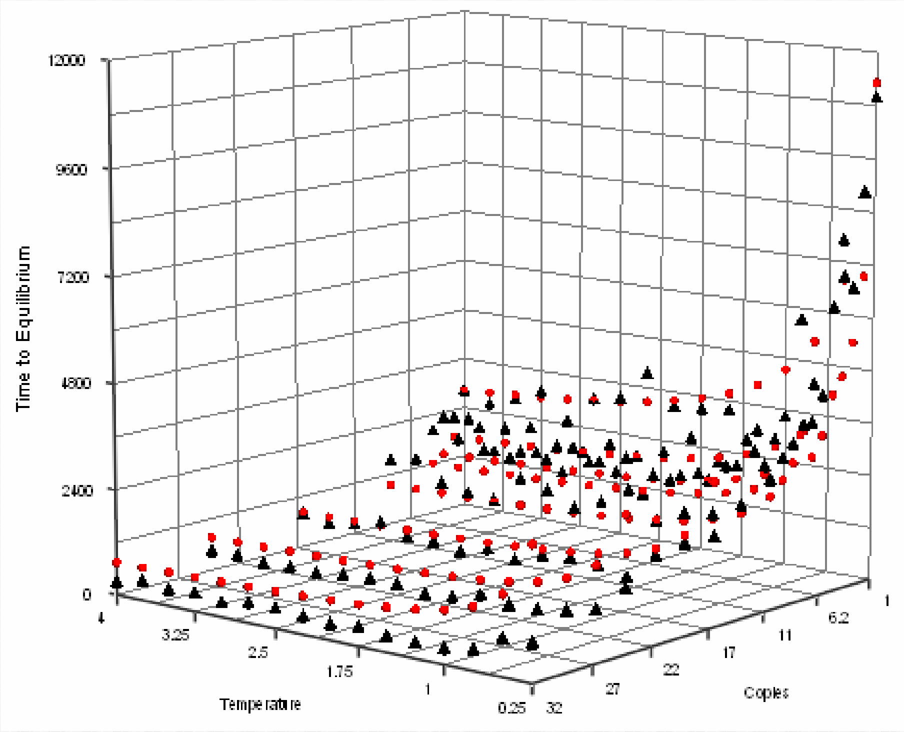
Predictive formulae

- $t_{\varepsilon}(T, N) = ((1/T) + 1) * ((1726/N) + 637.33)$



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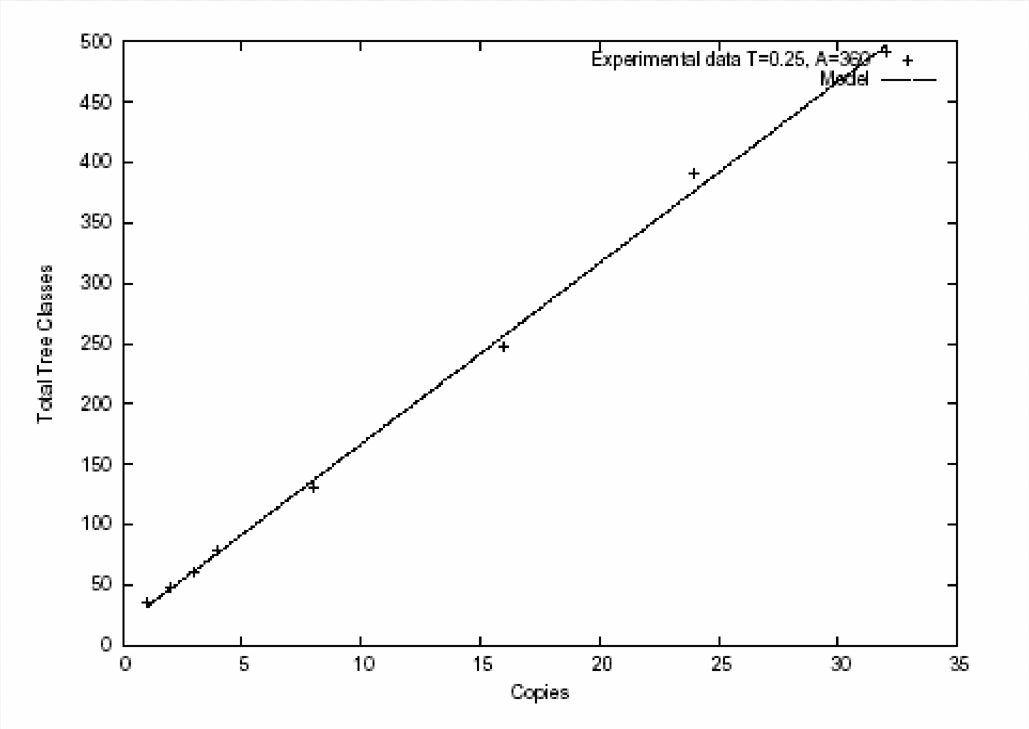
Predictive formulae

- $D_\varepsilon = 15*N + 16.6$



Prediction model assessment

equation	category	average error rate	standard deviation
Eq. 2	A=160	0.208	0.148
	A=250	0.425	0.525
	A=360	0.389	0.473
	A=490	0.261	0.374
Eq. 3	A=160	0.242	0.145
	A=250	0.152	0.146
	A=360	0.192	0.098
	A=490	0.097	0.090
Eq. 4	N=1	0.106	0.106
	N=2	0.129	0.089
	N=3	0.181	0.108
	N=4	0.263	0.095
	N=8	0.224	0.144
	N=16	0.219	0.189
	N=24	0.733	0.207
	N=32	1.190	0.521
Eq. 5	N/A	0.039	0.010

Conclusion

- In this talk, we have:
  - introduced an unguided software self-assembly system.
  - used kinetic theory on perfect gases as a metaphor for embodying $ASAP^2$.
  - from the experiments, we measured efficiency of software self-assembly and diversity of the generated programs.
  - obtained a suitable range of environment settings.
  - produced predictive equations for T_ε and D_ε
  - this prediction has not been done yet for GP.

Thank you!

Questions?