2013 YCCSA SUMMER SCHOLARSHIP PROJECT SUBMISSION

This form is for prospective project supervisors to submit their projects to be included in the YCCSA Summer Scholarships Programme for 2013.

It is the purpose of the Summer School that any projects submitted are interdisciplinary in nature.

Date	*15 Feb 2013*
Main Supervisor's Name	*Prof Susan Stepney*
Main Supervisor's Department	*Computer Science*
Co-supervisors' name(s) and Departments	*Dr Angelika Sebald* *Chemistry*
Project Title	***Adding Geometry to Artificial Chemistries***
Project Description	Artificial Chemistries (AChems) are abstract computational models built on analogies of real-world chemical reaction systems and networks. One aim is to provide a means of generating computational novelty, to provide a computational substrate for Artificial Life. Most AChems in the literature are naïve with respect to real chemistry, in particular, with respect to geometry. The electronic structure of real atoms is modelled by spherical harmonics as derived from quantum mechanical models. AChems include topology in their constraints (number of bonds and bonding graphs). However, no AChems explicitly include the concept of geometry, specific 3D constraints that require certain patterns of bond angles, etc. This project will investigate how to incorporate (an analogue of) geometry into a simple AChem, including consideration of spherical harmonics, and eigenvectors of matrix-based AChems, and build a small proof-of-concept system, to evaluate its usefulness.
Required skills	• Maths/physics knowledge of spherical harmonics of atomic orbitals • knowledge of eigenvectors • Programming ability
Project dates	*Monday 15 July 2013 -- Friday 13th September.*
Other information	
References	P. Dittrich, J. Ziegler, W. Banzhaf. Artificial Chemistries - A Review. *Artificial Life* **7**(3):225-275, 2001 doi:10.1162/106454601753238636

When complete, please email the form to sarah.christmas@york.ac.uk