1. INTRODUCTION

The EvoGrid, or EvoGrid, is an open, distributed artificial chemistry simulation grid now under development (Damer et al., 2010). The EvoGrid is designed to bring industrial scale simulation to bear on problems in origin of life endeavors including the modeling of da novo emergence of structures and reaction sequences in a prebiotic chemical milieu (Figure 1). Initial trials of the EvoGrid prototype constructed by a team at California based company DigitalSpace are presented here. The EvoGrid can enable distributed processing of any artificial chemistry simulation engine. The GROMACS molecular dynamics (MD) code was selected for the first tests due to its use in bio-relevant simulations such as Folding@Home (Pande et al., 2003). These in silico experiments are predictive and useful for chemists working in vitro based on the direction set by (Bedau et al, 2000) in the open questions in Artificial Life.

2. MODELS & METHODS

Due to the extreme computational costs involved in MD simulations, the EvoGrid focuses on simulating large numbers of small volumes containing 1K-10K atoms and employing search functions to select promising numbers of small volumes containing 1K-10K atoms and then placed in priority queues for continued simulation or abandonment.

3. IMPLEMENTATION

Figure 4 illustrates how simulation volumes are processed first by engines (such as GROMACS) then passed through analysis, searched and then placed in priority queues for continued simulation or abandonment.

4. RESULTS

Figure 5 illustrates the results of two experiments in which the search function (the teleological goal) was the formation of larger numbers of molecules from an atomic soup. In Experiment #1 a total of 66 molecules were formed within 1K atom volumes after two months of computing time on a small grid of 4 servers. 187 1K atom simulations were processed through 1,000 time steps, while 11,015 simulations were abandoned. In Experiment #6 with a modified search function permitting the discovery of higher maxima 144 molecules were observed through 966 processed and 61,415 abandoned. In a control experiment, 26 molecules where observed but there was no sustained trend: no ability to sustain a local maximum and search for a higher one.

5. CONCLUSIONS

The EvoGrid is designed to bring industrial scale computing to origin of life experiments such as simulating the emergence of lipids and their association into micelles or vesicles, the arising of auto-catalytic sets, and scenarios for polymerization and replication of informational molecules. The following roadmap is proposed for future EvoGrid implementations beyond the current prototype (Damer, 2011). These simulation targets are listed in order of perceived difficulty and provide a ten to twenty year time horizon for the ability of computation to handle the suggested volumes over bio-relevant time scales.

LITERATURE CITED


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