

Molecular Dyna-Cloud, 5/09/2012

“D99: Gabriel Dunham”

Problem Definition

- Problem Statement

It is difficult to study molecular structures especially as they respond to forces

- Scope

Create the interface between the EC2 instance *and*

Research efficiency of data transmission

- Schedule

Spring: Research and Test Communications

Summer: Complete Prototype Simulation Interface

Fall: Complete Self Sustained Implementation

- Resources

Java, C, and Eclipse/NetBeans

Test Server

EC2 Instance

*See data sheet for more information on resources.

Research/Analysis

There are many groups working on similar problems.

- IBM and Google's Cloud computing Initiative is researching feasibility and efficiency.
- StACC, the Computer Science Division at the University of St Andrew's
- North Carolina State University is researching possible implementations of a “trustworthy” cloud.

Proposed Solution

The solution which this project will employ is to use an EC2 instance (Amazon's Cloud Computing service) to run the calculation-heavy simulations.

The purpose of this project is to design and implement a system by which these simulations may be transmitted to the EC2 instance.

In the long term, the goal is to eventually design a system which effectively allows a user to design code and move it to/receive data from the cloud.

Ideally, the user should not require large amounts of help from tech support in order to load/run simple applications.

Potential Applications

- Molecular Dynamics Simulations
- Unified Software Distribution throughout a Corporation
- Anytime/Anywhere access to running applications
- A simple back up system for small companies
- General IT management solutions

