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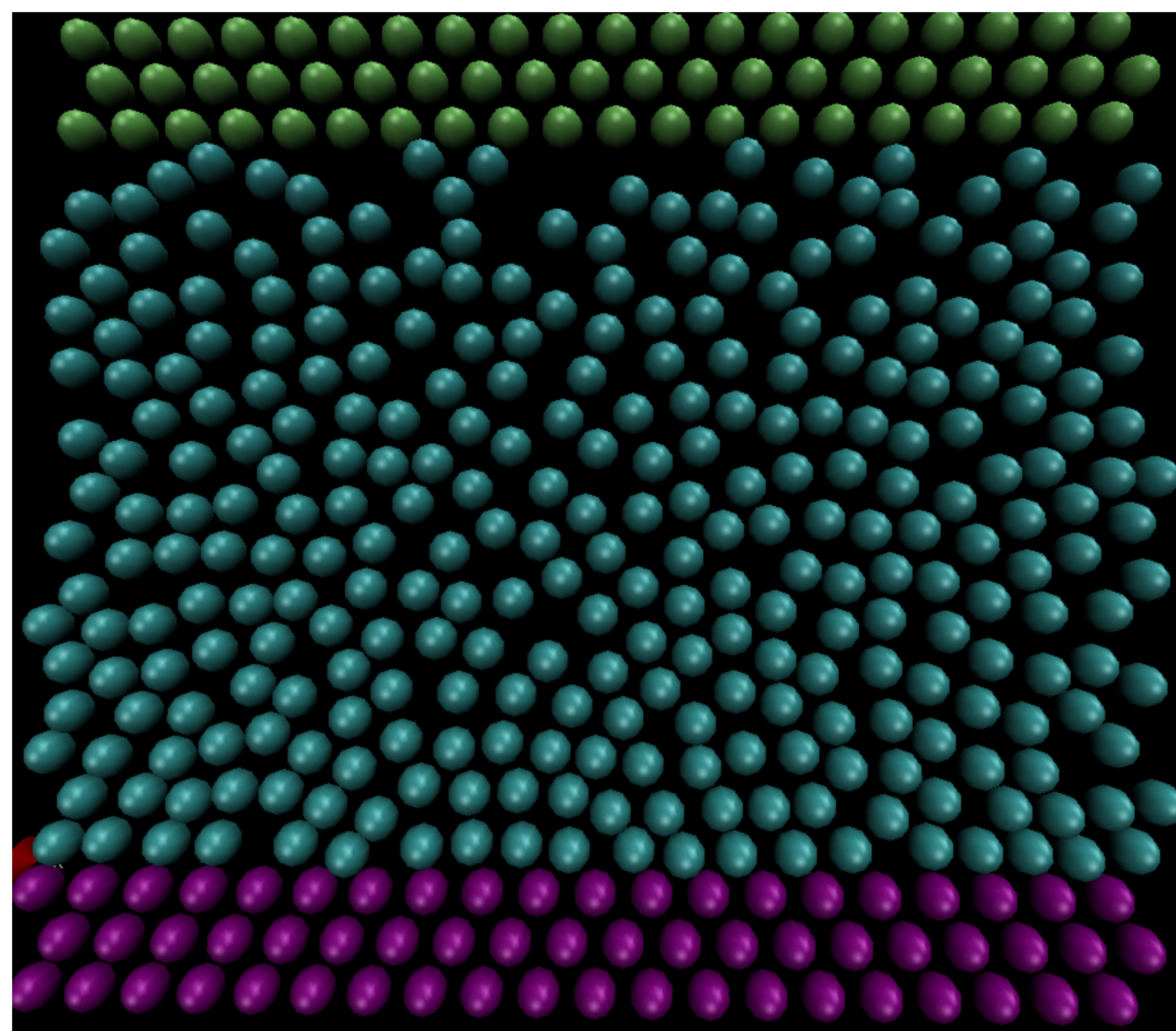
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Background

- Molecular Dynamics Simulations let you observe molecules
- But simulations take a lot of time and money
- Can we speed things up by using high-performance cloud computing technology?



Typical Solution

Computer Clusters

- Uses a lot of computers
- Usually close together
- Really expensive.

Objectives

- Derive a mathematical and experimental model for these cloud-simulations
- Determine whether or not it's beneficial to use multiple cloud computing instances
- Create a system that divides the work up efficiently between cloud computers

The Molecular Dyna-Cloud System

The Hardware and Software

- Amazon's Elastic Cloud Compute Unit (EC2 instance)
- Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)
- Visual Molecular Dynamics (VMD)

System Setup

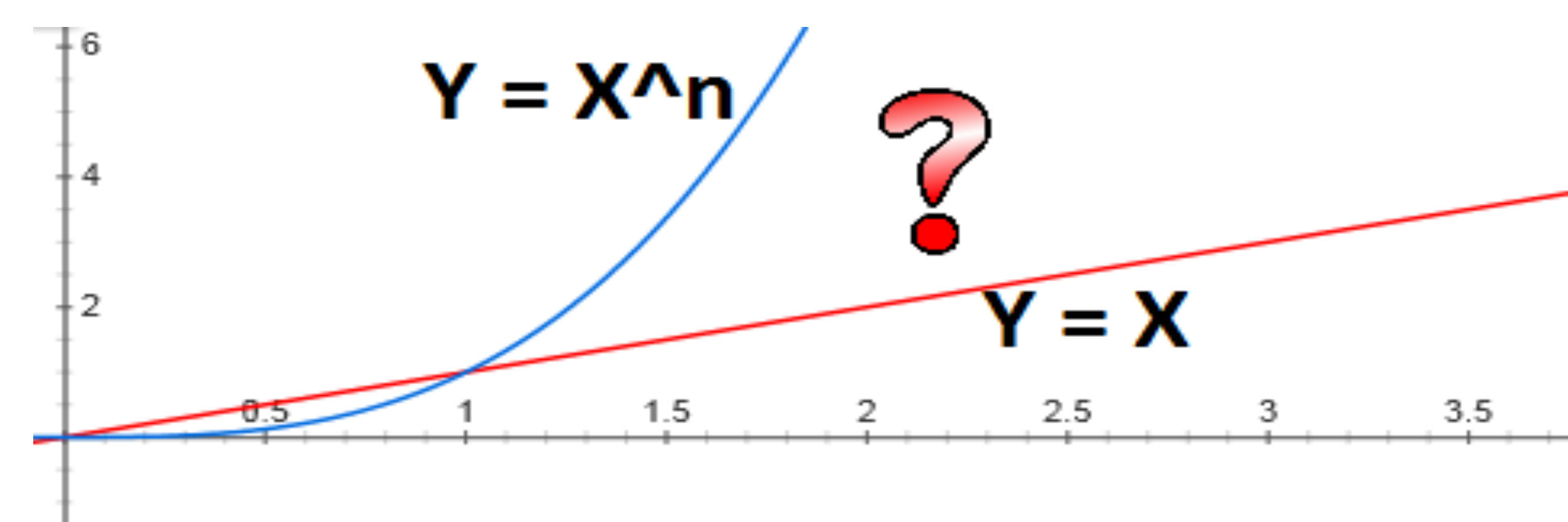
- Simulation is divided into regions
- Each EC2 simulates a region
- The EC2's 'talk' to each other after each 'step'



Experiments

1) Determine the increase in communication-time with respect to the size of a simulation

- As the number of EC2 instances increases, so does the amount of time spent communicating
- Conduct experiments to determine what relationship exists between the size of a simulation and the time spent communicating

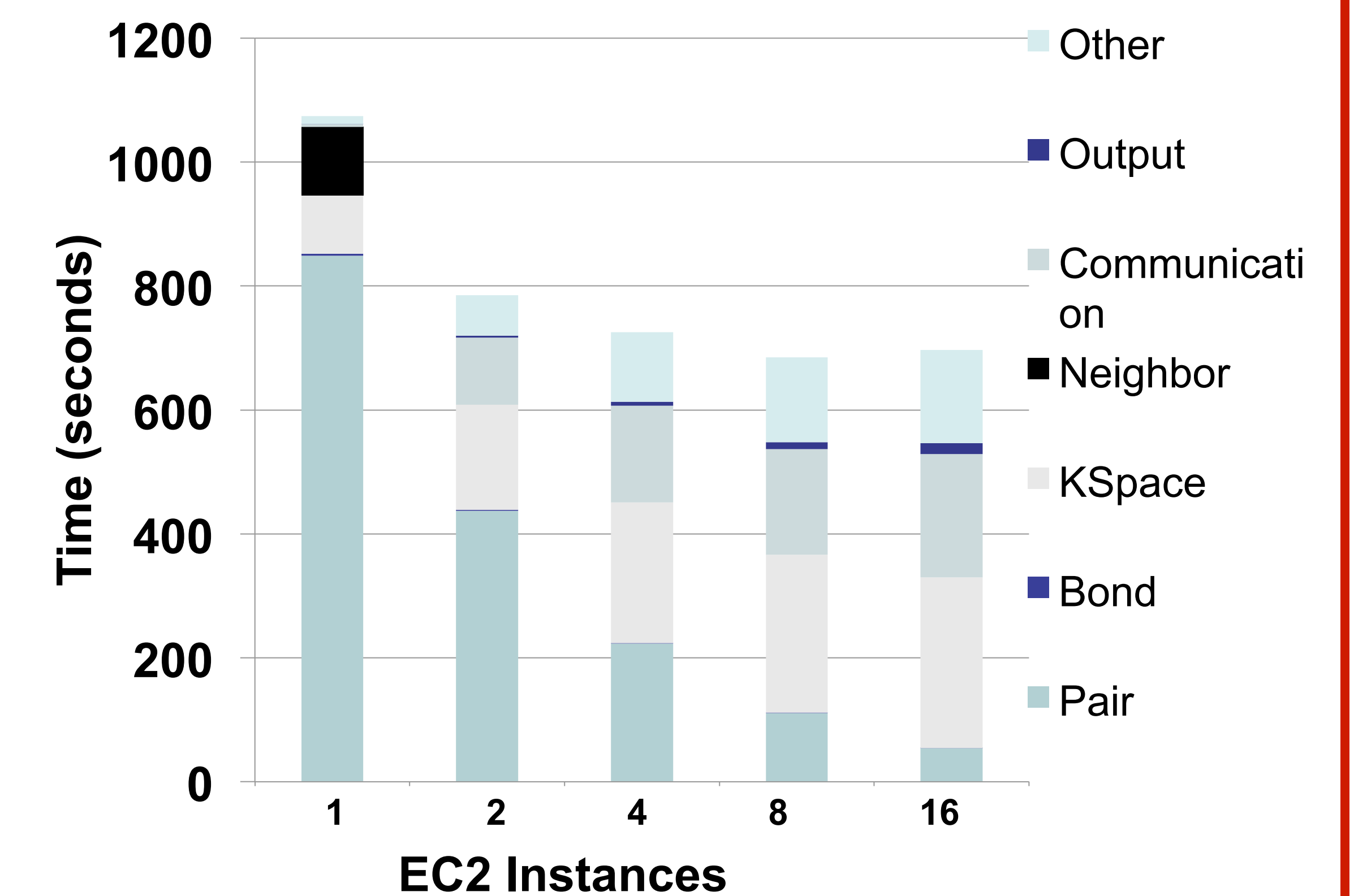


2) Determine the decrease in total-time with respect to the number of EC2 instances

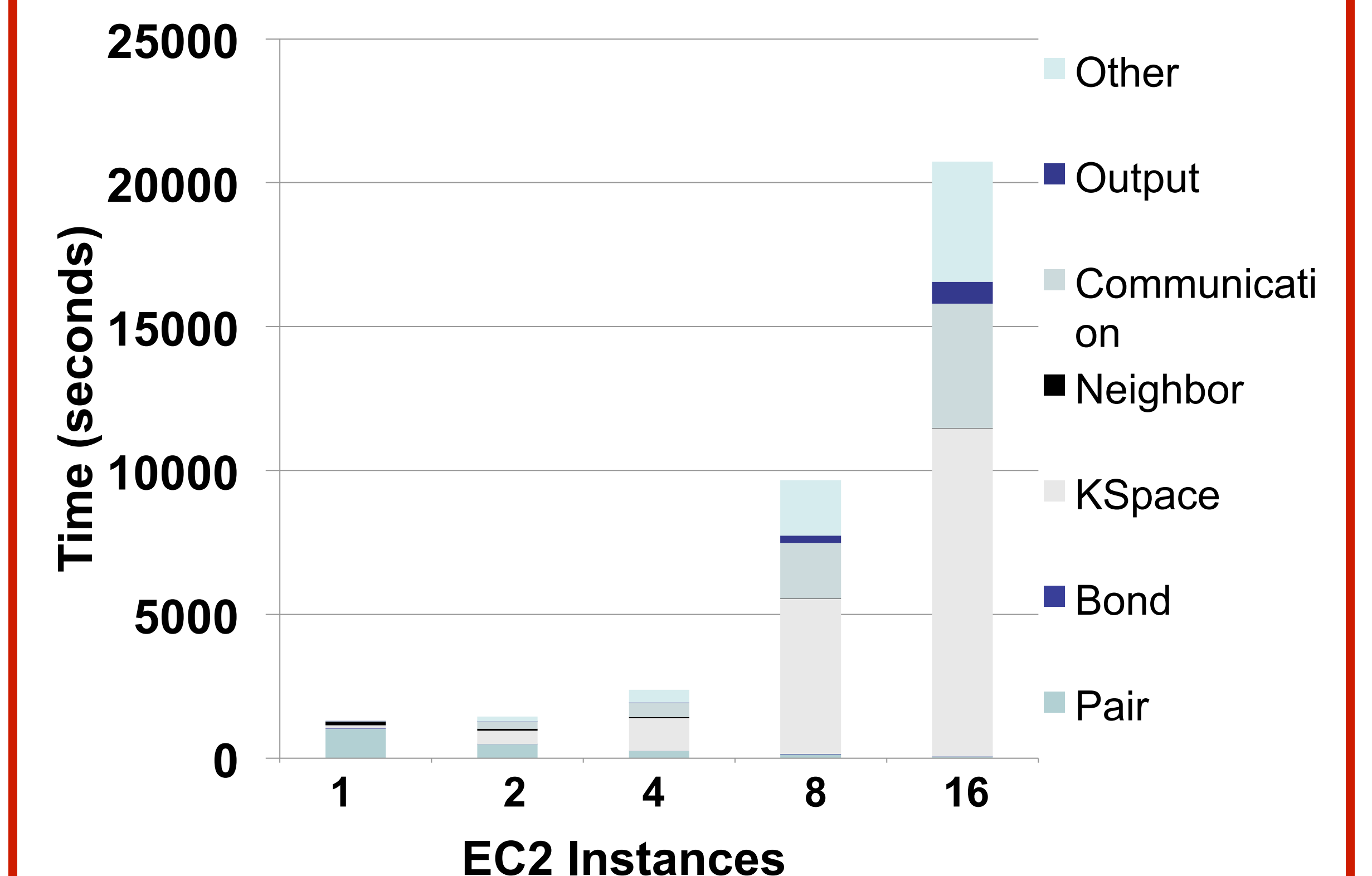
- It is predicted that the amount of time that a given molecular dynamics simulation requires is directly related to the number of EC2 instances
- Experiments are being conducted to find the relationship between the number of EC2 instances and the time that a simulation takes

Early Results

Time vs. # of Instances



Time vs. # of Instances



Conclusions

- The Molecular Dyna-Cloud System seems to be feasible
- Communication-time could be a big problem for small simulations
- The location of each EC2 instance seems to have a large affect on communication-time

Acknowledgement

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