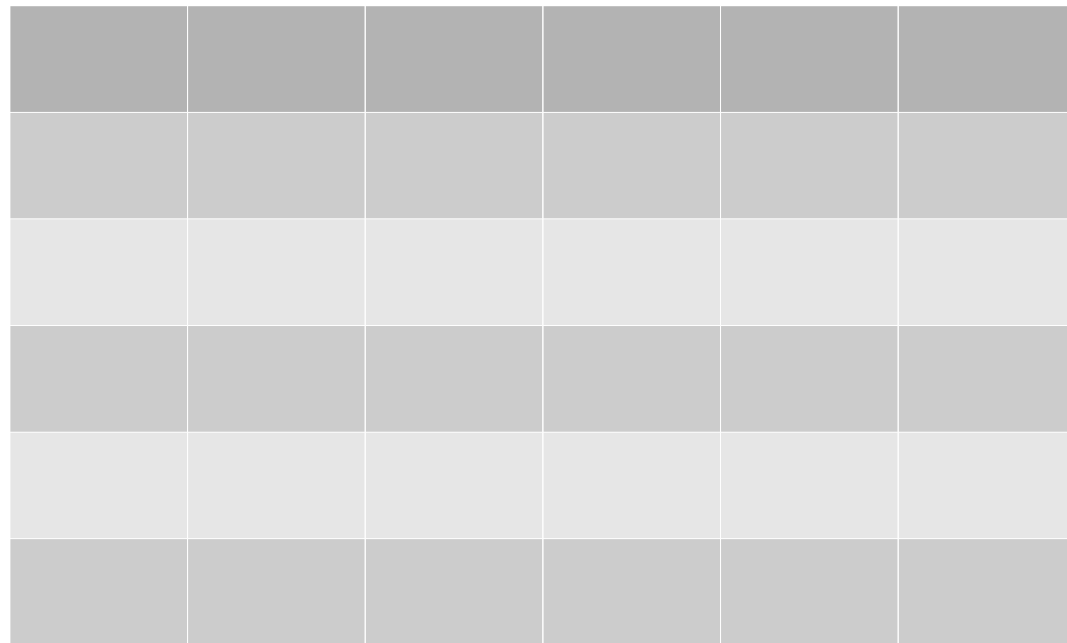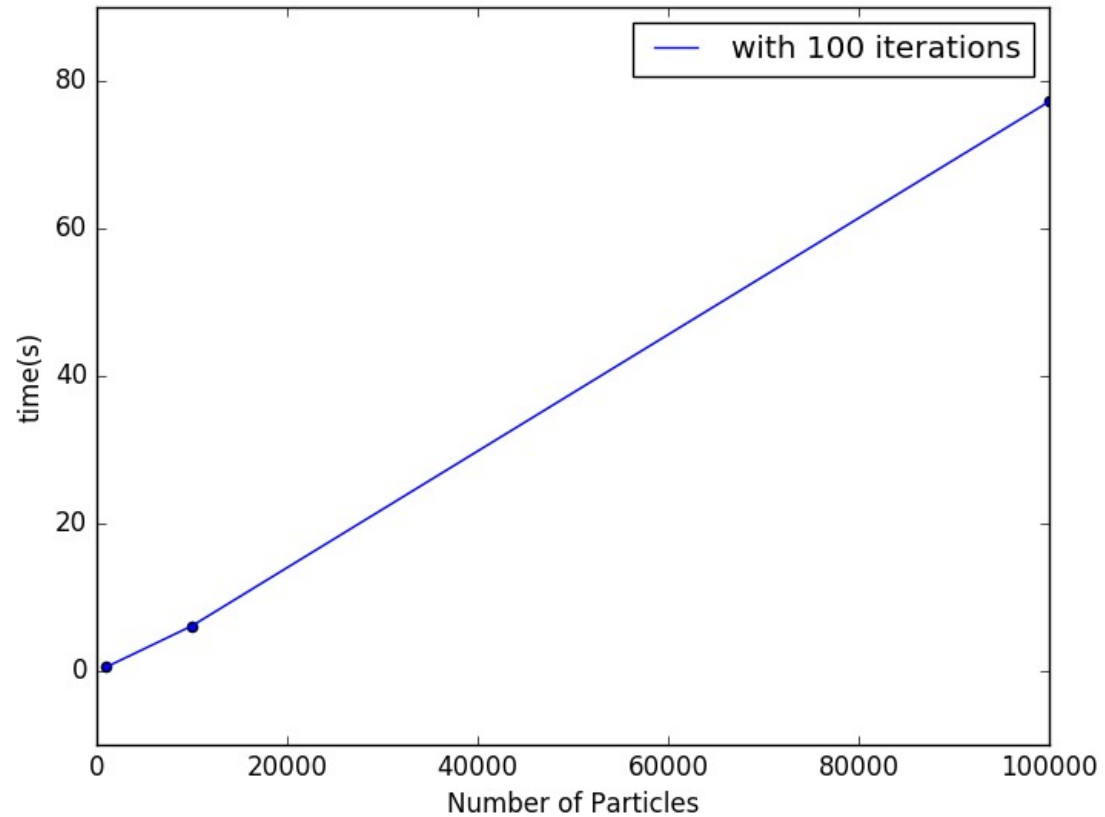# Molecular Dynamics Project

Sandeep Kumar Kataria
14 October, 2016
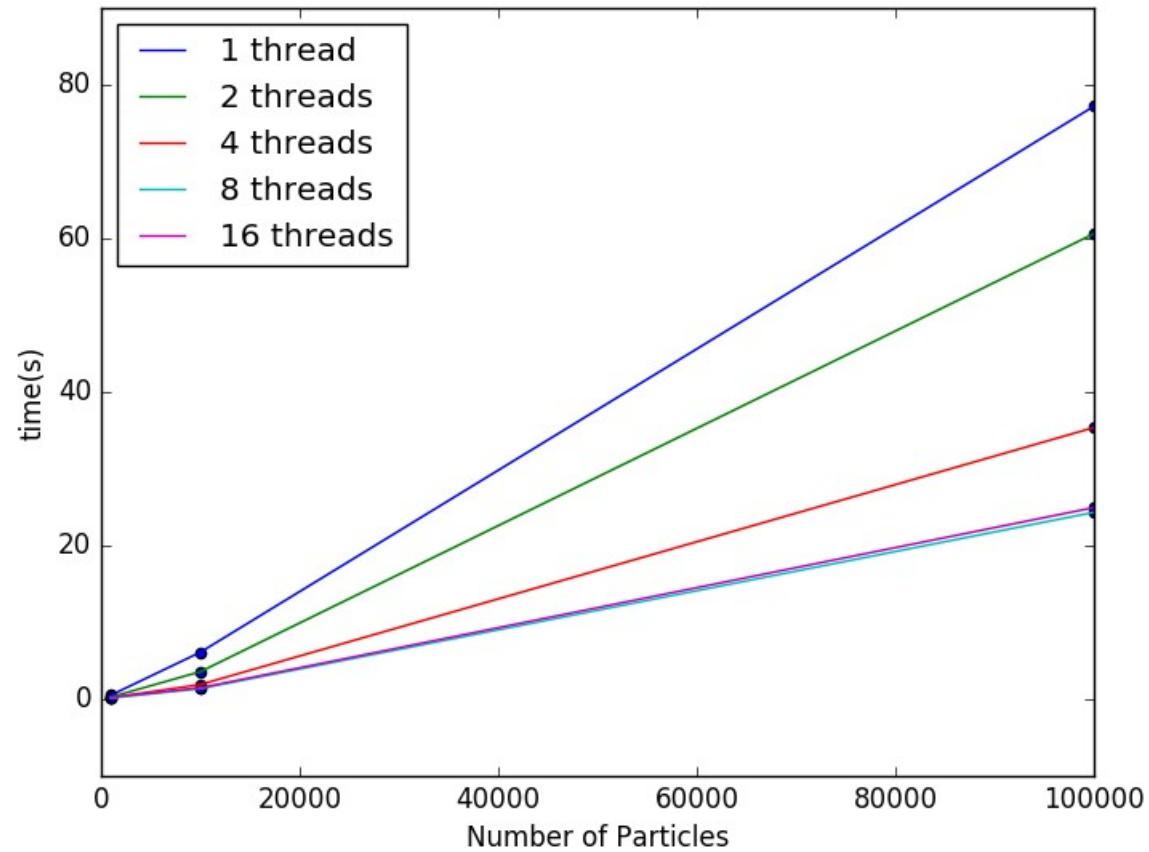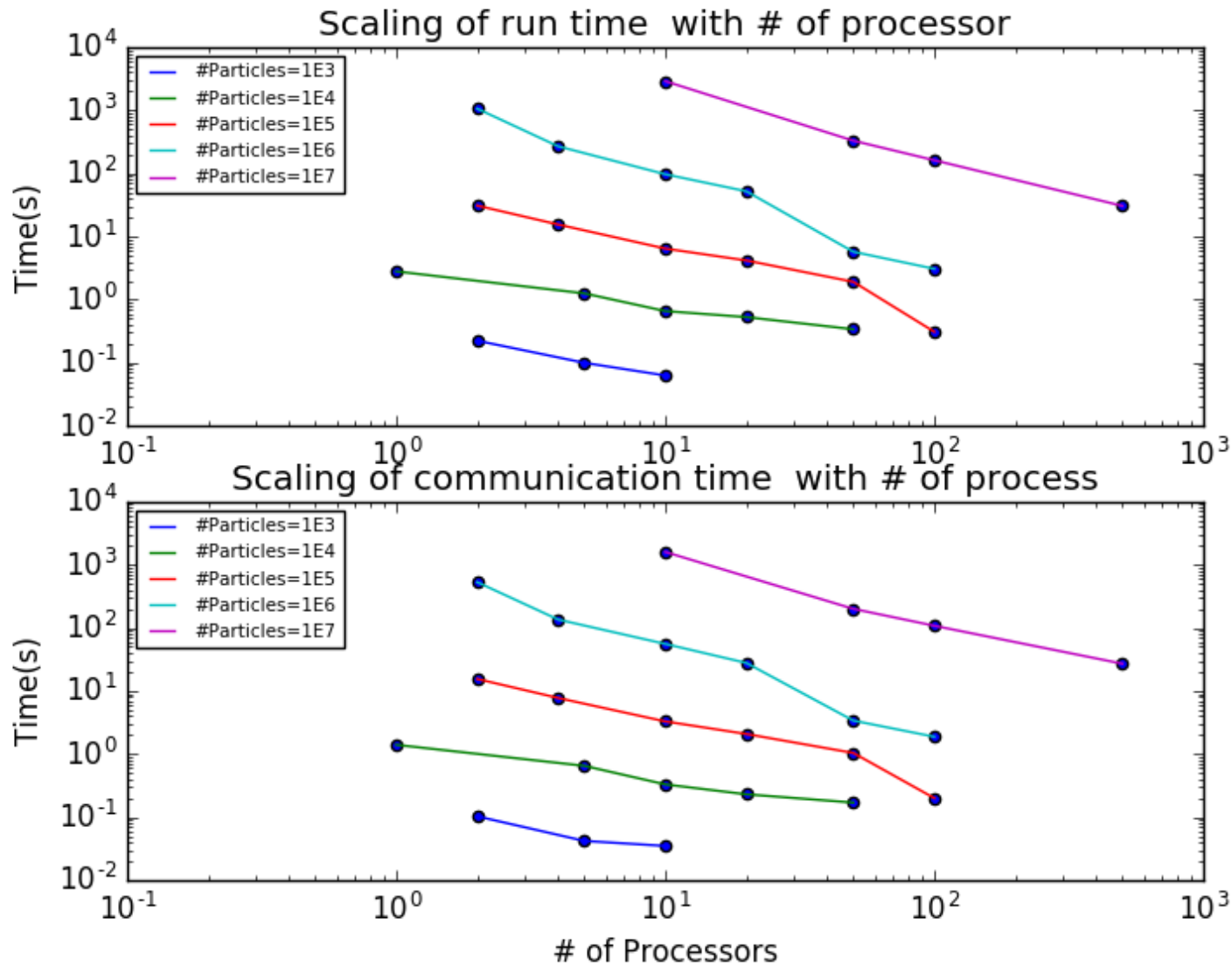
Introduction

Serial Code Scaling

Running using OpenMP

Running With MPI

Conclusion

- Serial Problem scales inbetween linear and square of number of atoms. It is bounded by memory of system as number of particles increases.

- With OpenMP with increasing number of threads we can get speed but still bounded by system with increasing number of particles(shared memory).

- In MPI with increasing number of processes time run time reduces to significant amount. In our case communication time is almost matched by calculation time.