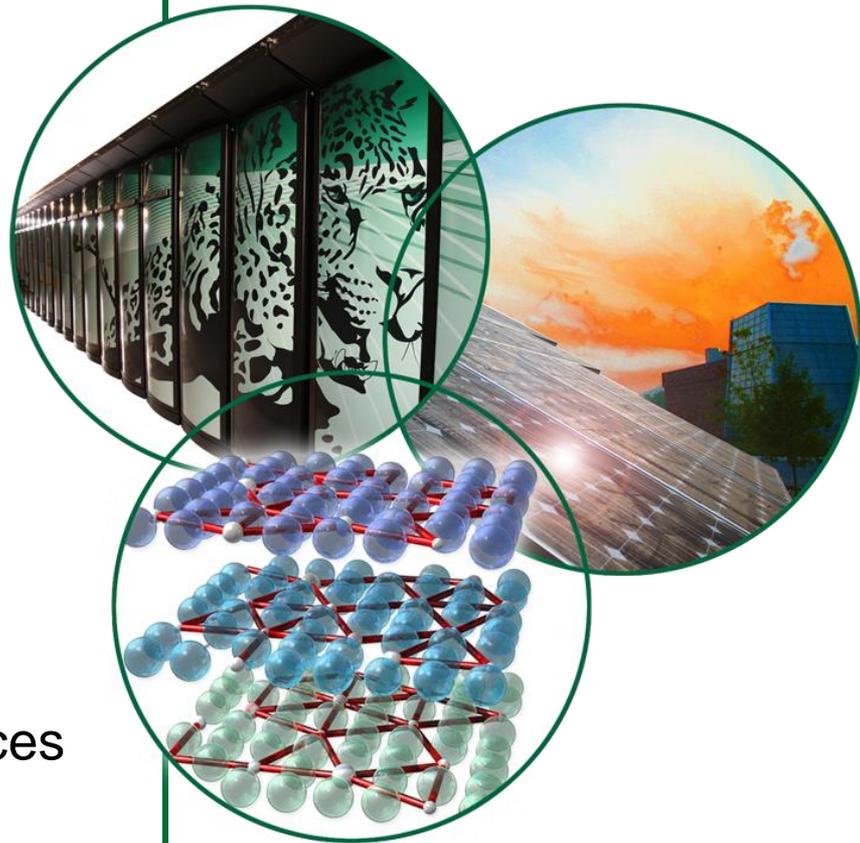


Performance for Profiling Molecular Dynamic Codes

Justin Vaughner
Alabama Agricultural and Mechanical
University

Arnold Tharrington PhD
Scientific Computing Group
National Center for Computational Sciences

August 2009



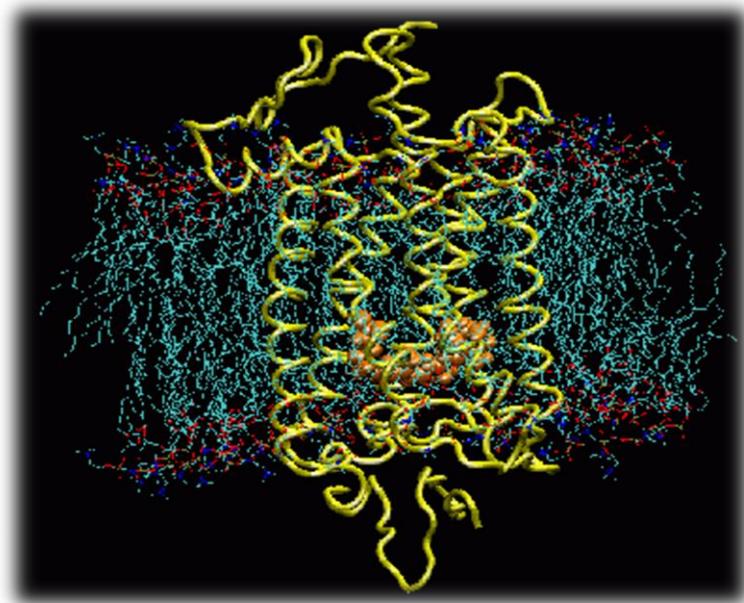
Overview

- **Introduction**
- **Background Information**
- **Methodology**
- **Results**
- **Conclusion/future work**
- **Acknowledgments**

Introduction

- Understand and optimize algorithm performance in Large atomic/Molecular Massively Parallel Simulator (LAMMPS) Molecular Dynamics (MD) code XT5 architecture (JaguarPF)
- Rhodopsin biological system will be used in this computational performance study
 - Protein found in the retina of the eye
 - ~ 30,000 atoms →

- Rhodopsin
- Retinal
- Water molecule



JaguarPF(XT5) supercomputer



- **XT5 contains 18,688 (149,504 cores) compute nodes.**
- **Compute node contains two quad-core AMD Opteron 2356 processors running at 2.3 GHz**
- **16GB of DDR2-800 memory**
- **SeaStar 2+ router**
- **Peak performance of 1.38 petaflop**
- **Operation cost- \$1,000,000 per day**

What are petaflops?

- 1.38 petaflops (1.38 quadrillion floating point operations per second)
 - Human $1.1+1.1=2.2$ “1 flop per second”
 - 3600s = flop per hour
 - $3600s*24= 86400$ flops per day
 - $86400s*365=31536000$ /flops per year
 - ~ 31,000,000 years

Methodology of project

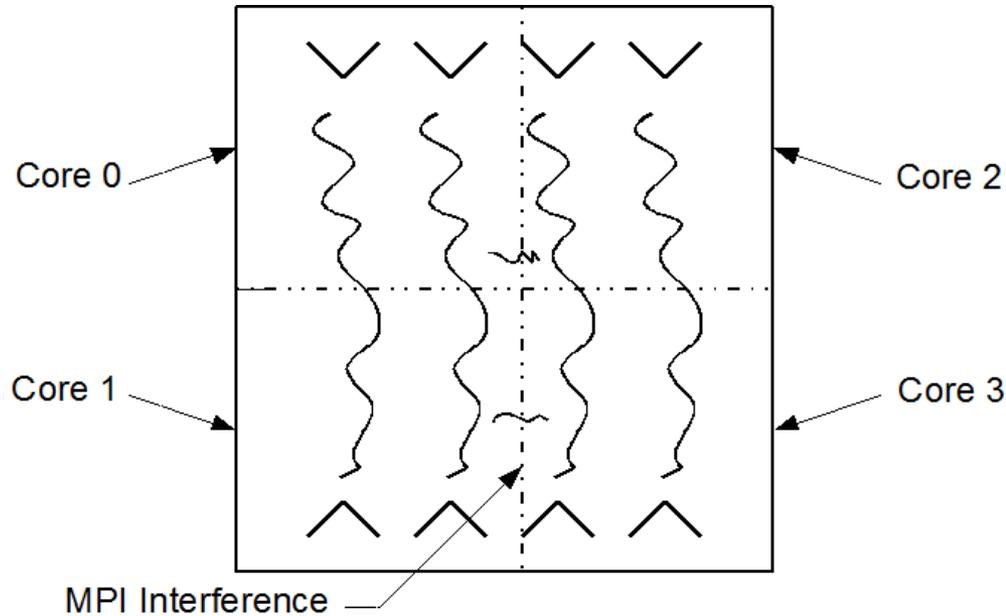
- **UNIX operating system**
 - **bash shell**
 - **vi editor**
 - **Molecular dynamics**
 - **Message passing Interface (MPI) programming**
- **Craypat- performance tool to use profile MD codes**

What are Molecular Dynamics (MD) Codes?

- MD codes used to perform atomistic computer simulations of materials and/or biological systems (LAMMPS)
- MD codes to compute forces of atoms interacting with each other in a given biological system
 - Newton's second law of motion

Domain decomposition use by LAMMPS

- Domain decomposition
 - Spatial decomposition
 - Newton's second law of motion

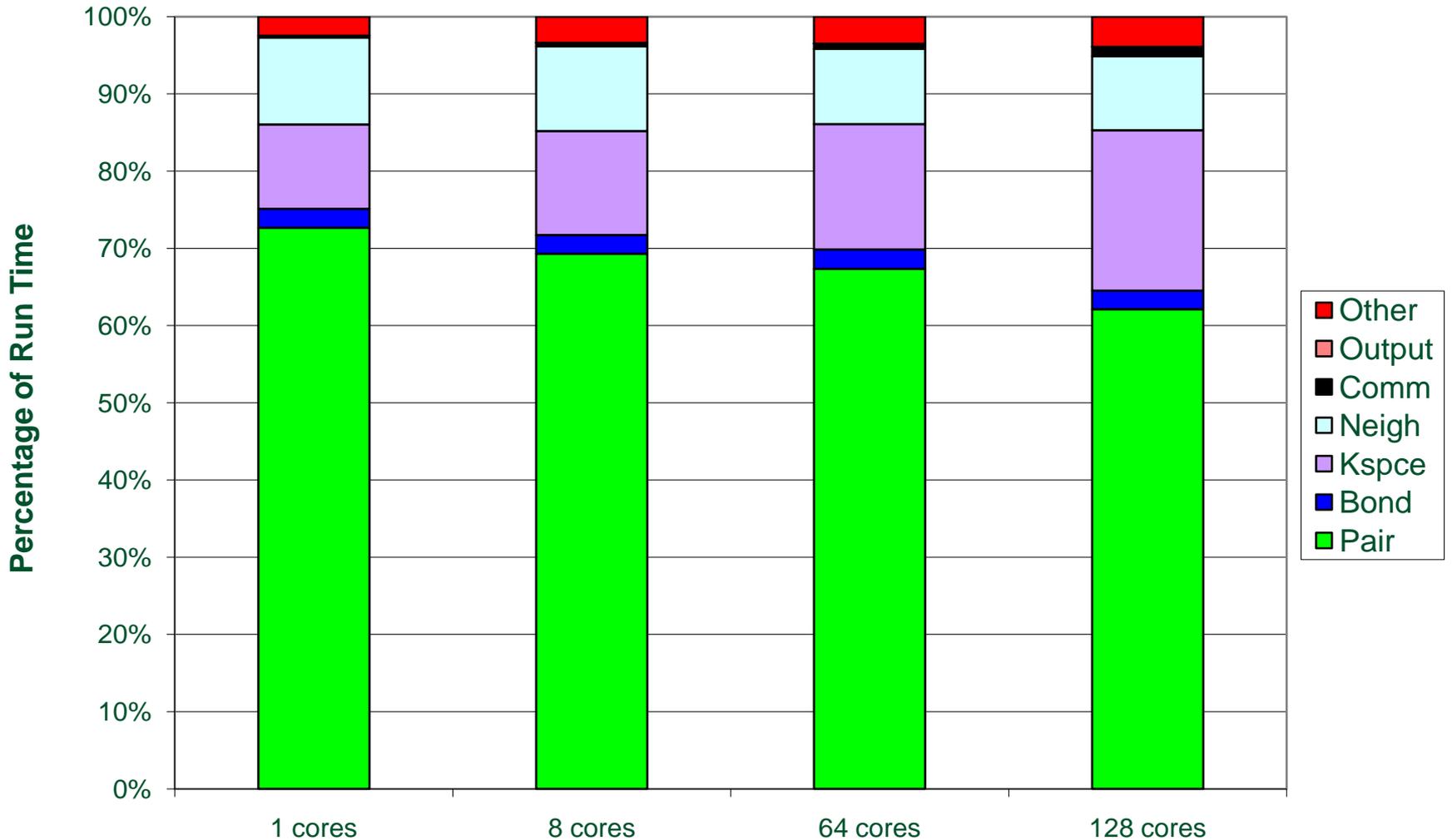


$$\vec{F} = m\vec{a}$$

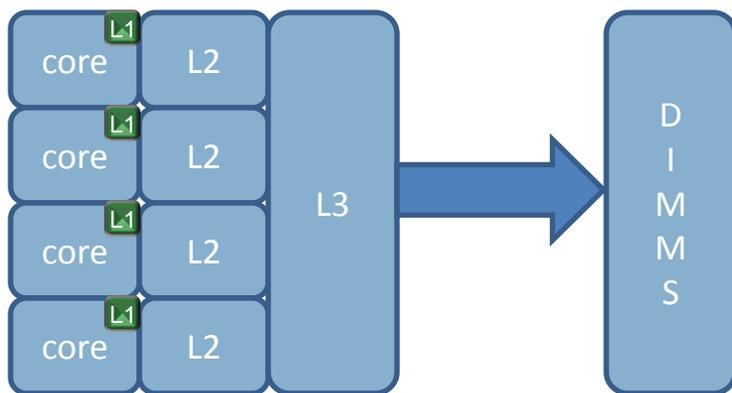
$$\vec{F}_{Net} = \vec{F}_{Bonds} + \vec{F}_{Angle} + \vec{F}_{Dihedral} + \vec{F}_{Columbic}$$

Plot time vs. Number of cores

Time spent in each part of LAMMPS

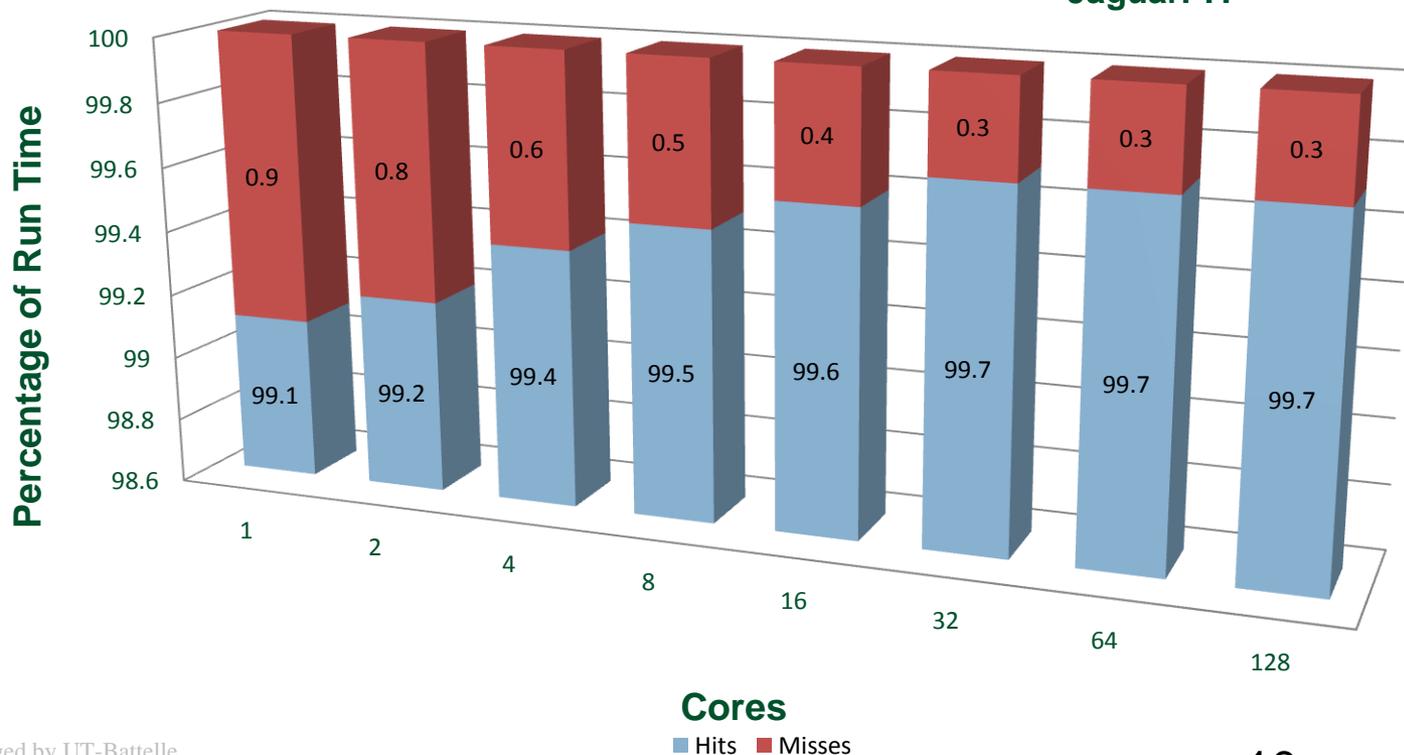


Level 1 and 2 cache hit and miss ratio

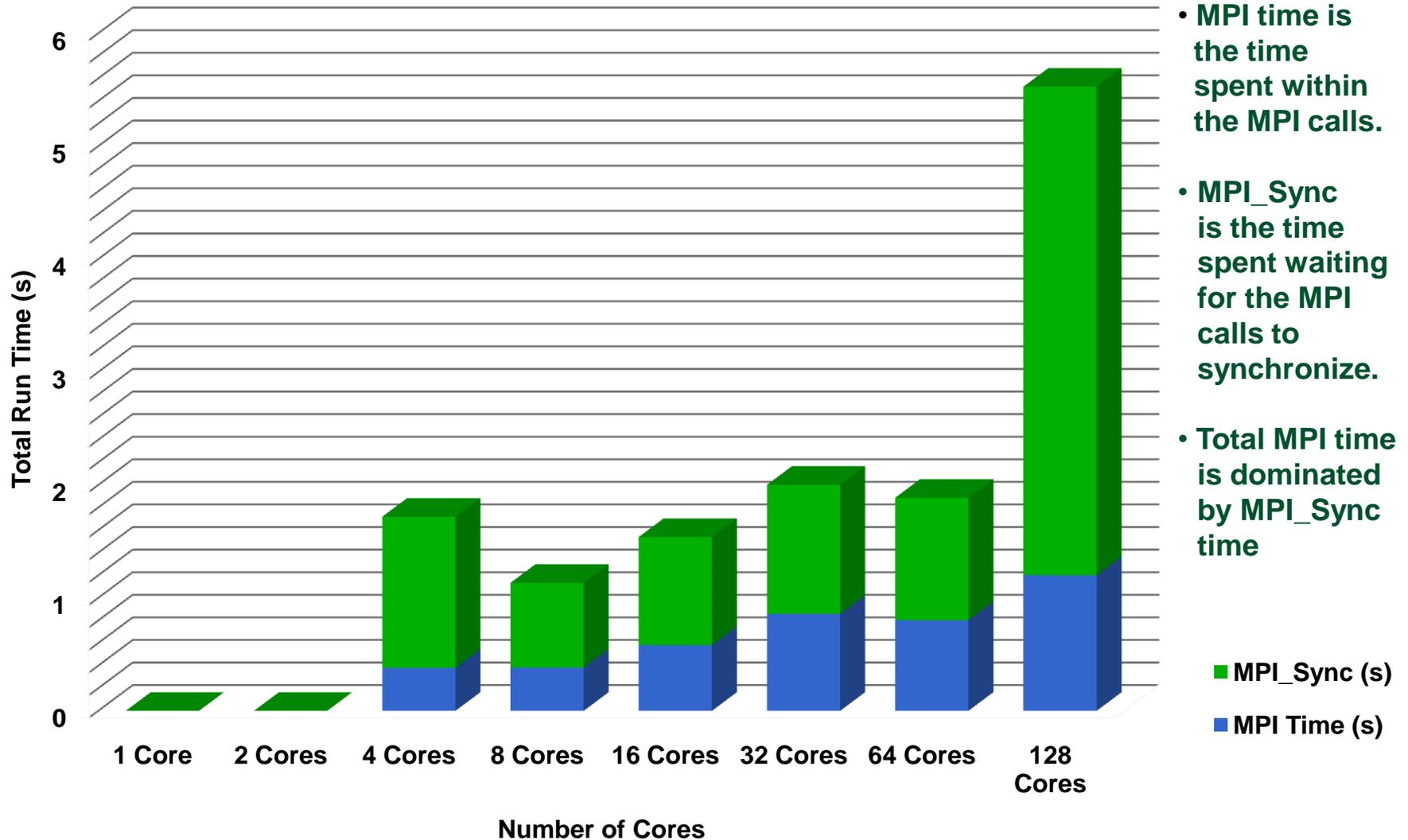


Information is searched in Levels 1, 2, 3, and DIMS. If information is not found in one level, it misses and goes to the next level.

LAMMPS cache hit and miss ratio remains constant with the number of cores while running on JaguarPF.



MPI and MPI SYNC



- MPI time is the time spent within the MPI calls.
- MPI_Sync is the time spent waiting for the MPI calls to synchronize.
- Total MPI time is dominated by MPI_Sync time

■ MPI_Sync (s)
■ MPI Time (s)

Conclusion

- **Observed and understood how an MD code interacts with the supercomputer**
- **Code will be modified for optimized performance on supercomputer**
- **Process will be performed on future supercomputer projects**
 - **Six -core Upgrade (Istanbul)**
 - **Future Hybrid Graphics Processing Unit (GPU) Supercomputer**

References

- **Plimpton, Steve. “LAMMPS Molecular Dynamics Simulator.” 1995. Sandia National Laboratory. <http://lammps.sandia.gov/>**
- **K. Palczewski et al., Science 289, 739 (2000). <http://www.ks.uiuc.edu/Research/rhodopsin/>**

Acknowledgments

- **Mentor- Arnold Tharrington PhD**
- **RAMS Director- Debbie McCoy**
- **Research Alliance in Math and Science (RAMS)**
- **National Center of Computational Science**
- **Department of Energy (DOE)**
- **National Science Foundation (NSF)**