PPL Mission and Approach

- To enhance *Performance and Productivity* in programming complex parallel applications
  - Performance: scalable to thousands of processors
  - Productivity: of human programmers
  - Complex: irregular structure, dynamic variations
- *Application Oriented yet CS centered research*
  - Develop enabling technology, for a wide collection of apps.
  - Develop, use and test it in the context of real applications
  - Embody it into easy to use abstractions

Parallel Programming Laboratory

- Senior Staff: 4
  - Res. Scientist: 1
  - Res. Programmer: 1
  - Postdoc: 2
- Grad Students (RAs): 10
- Undergrads: 1
- Software distributed
  - Charm++
  - AMPI
  - NAMD (with K.Schulten)
  - ChaNGa (with T.Quinn)
  - ParFUM
- Approx. annual funding
  - ~ $1.0 M

- Claim to fame:
  - Most widely used academically generated parallel programming system
    - (suggested by Jim Browne)
  - Gordon Bell Award, 2002
    - Shared
  - One of the large groups in parallel computing
    - Becoming well-known
  - Known for intense collaborations
  - Auto. Runtime Optimizations
    - Dynamic Load Balancing
    - Communication optimizations

Parallel Programming Laboratory

Sr.STAFF





GRANTS

- NSF/NCSA Track-1: Blue Waters Petascale System
- NSF: ITR , NASA Computational Cosmology and Visualization
- DOE HPC-Colony Services and Interfaces for Large Computers
- NSF: ITR Chemistry Car-Parinello MD, QM/MM
- NSF: CSR-SMA Big System Simulation
- NIH Biophysics NAMD
- DOE CSAR Rocket Simulation
- NSF: ITR CPSD Space / Time Meshing

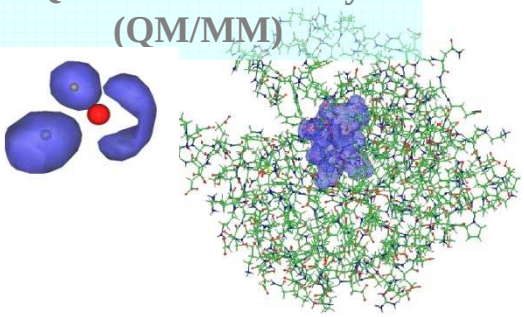
ENABLING PROJECTS

- **Faucets**: Dynamic Resource Management for Grids
- **Load-Balance**: Centralized, Distributed, Hybrid
- **Fault-Tolerance**: Checkpointing, Fault-Recovery, Proc.Evacuation
- **ParFUM**: Supporting Unstructured Meshes (Comp.Geometry)
- **BigSim**: Simulating Big Machines and Networks

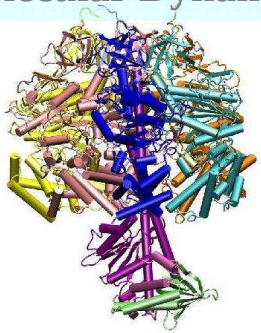
- Charm++ and Converse
- AMPI Adaptive MPI
- Projections: Performance Analysis
- Orchestration and Parallel Languages

Develop abstractions in context of full-scale applications

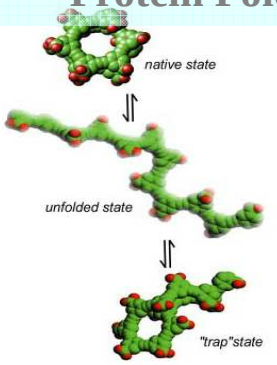
Quantum Chemistry (QM/MM)



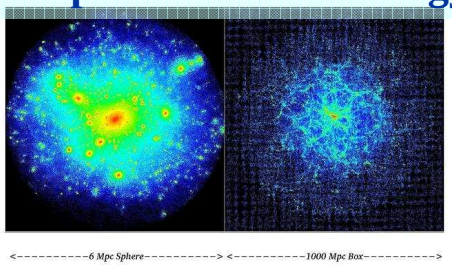
Molecular Dynamics



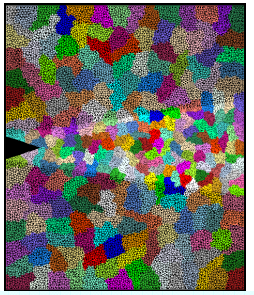
Protein Folding



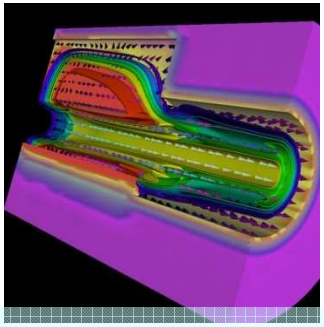
Computational Cosmology



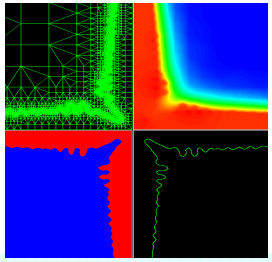
Parallel Objects,
Adaptive Runtime System
Libraries and Tools



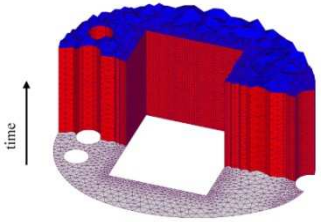
Crack Propagation



Rocket Simulation



Dendritic Growth



Space-time meshes

The enabling CS technology of parallel objects and intelligent runtime systems has led to several collaborative applications in CSE

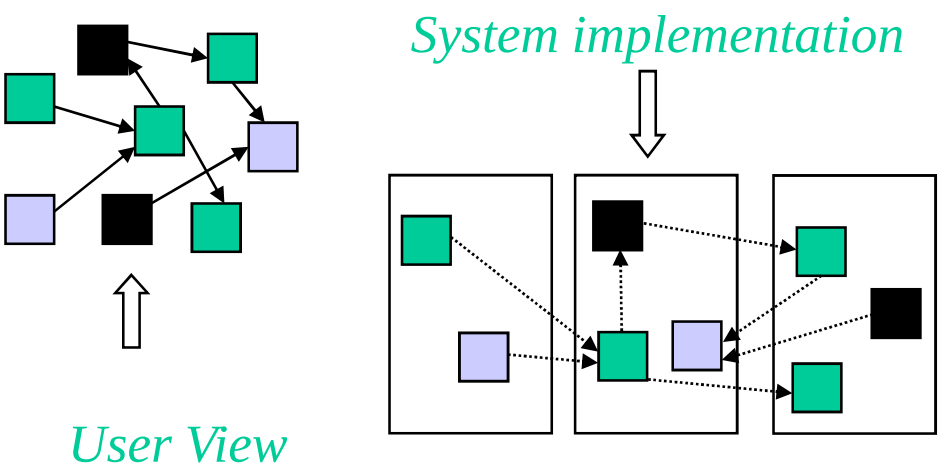
Migratable Objects (aka Processor Virtualization)

Programmer: [Over] decomposition into virtual processors

Runtime: Assigns VPs to processors

Enables *adaptive runtime strategies*

Implementations: Charm++, AMPI

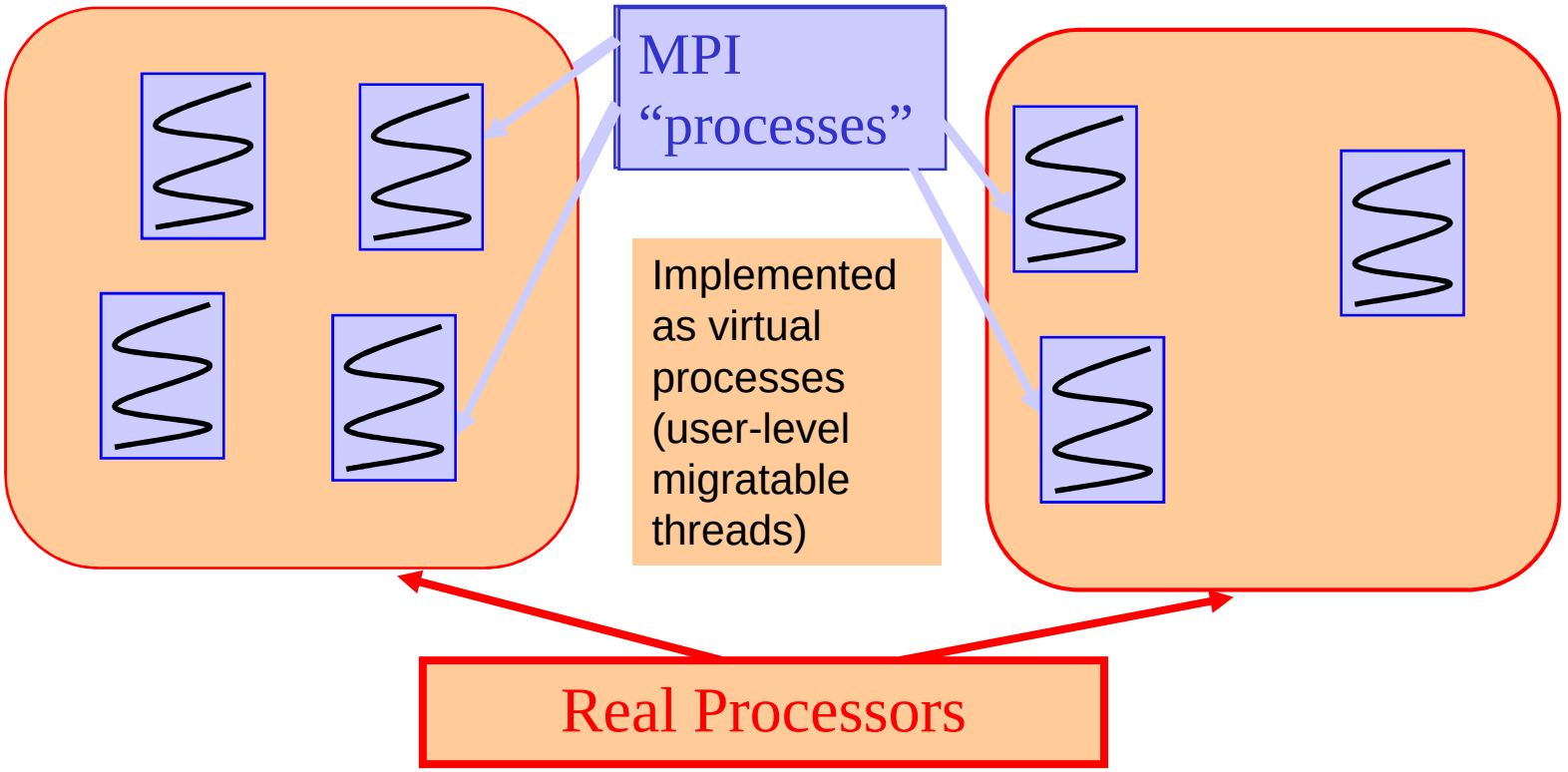


Benefits

- Software engineering
  - Number of virtual processors can be independently controlled
  - Separate VPs for different modules
- Message driven execution
  - Adaptive overlap of communication
  - Predictability :
    - Automatic out-of-core
  - Asynchronous reductions
- Dynamic mapping
  - Heterogeneous clusters
    - Vacate, adjust to speed, share
  - Automatic checkpointing
  - Change set of processors used
  - Automatic dynamic load balancing
  - Communication optimization

AMPI: MPI with Virtualization

- Each virtual process implemented as a user-level *thread* embedded in a Charm *object*



PPL Personnel

- CSAR (Rocket Center)
  - Postdocs:
    - Gengbin Zheng
    - Terry Wilmarth (0.5)
  - RAs:
    - Pritish Jetley
    - Abhinav Bhatele (0.5)
- Biophysics (Schulten)
  - RAs:
    - Chee Wai Lee
    - David Kunzman
    - Mei Chao
- Cosmology (Quinn)
  - RA: Filippo Gioachin
- Fellowships:
  - DOE - HPC: Isaac Dooley
  - Siebel Scholar: Lukasz Wesolowski
- Quantum Chemistry (CPAIMD)
  - Staff: Eric Bohm
  - RA: Abhinav Bhatele (0.5)
- CPSD:
  - Postdoc: Terry Wilmarth (0.5)
  - RAs:
    - Sayantan Chakravorty (0.5)
    - Aaron Becker (0.5)
- DOE/LLNL
  - Staff: Celso Mendes
  - RAs:
    - Sayantan Chakravorty (0.5)
    - Aaron Becker (0.5)
- NSF R.E.Undergrad:
  - Ekaterina Gonina