



Global Address Space Applications

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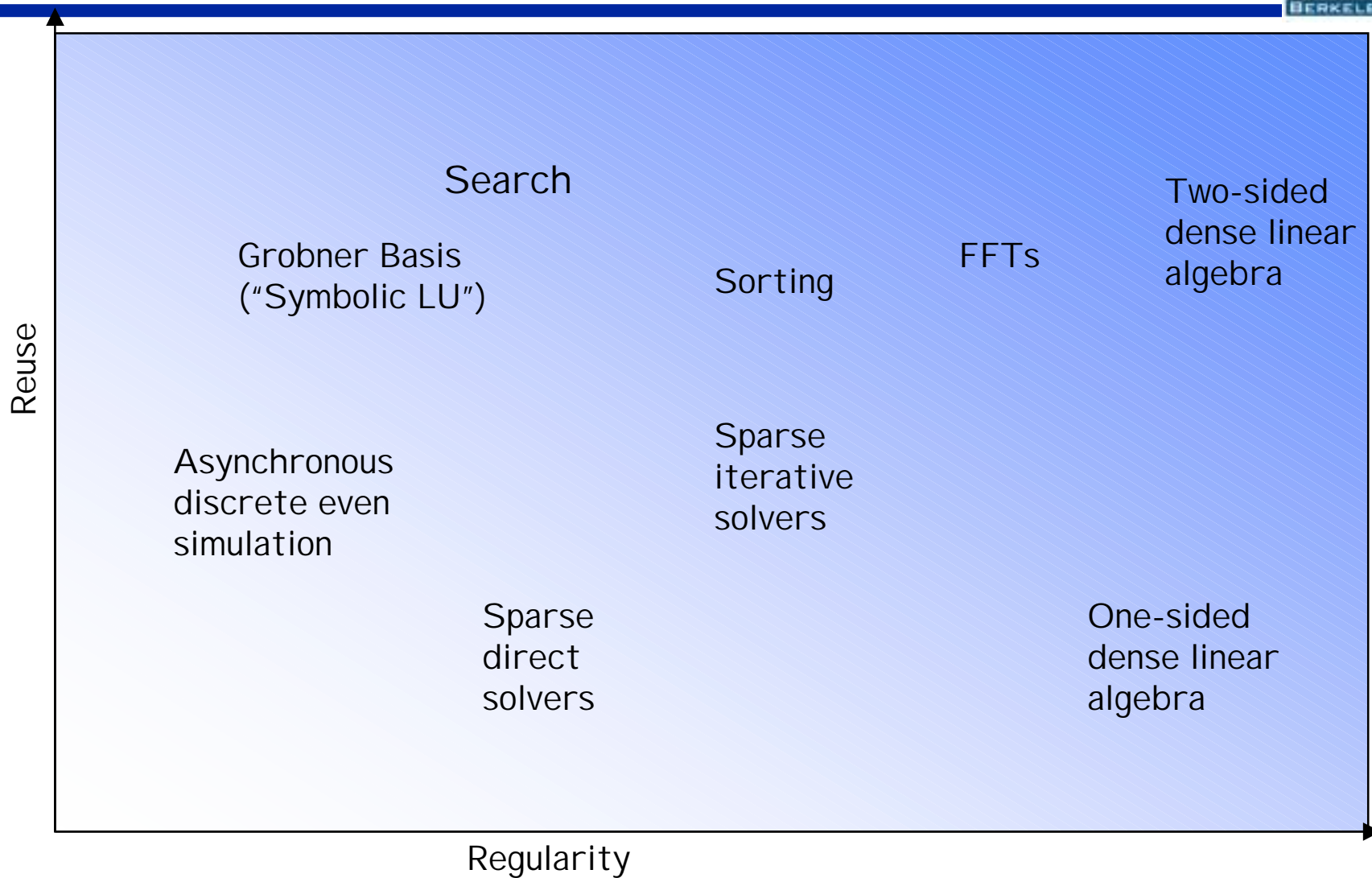
NERSC

**NATIONAL ENERGY RESEARCH
SCIENTIFIC COMPUTING CENTER**

**Advancing Computational Science of Scale—
Producing Real Results**



Algorithm Space

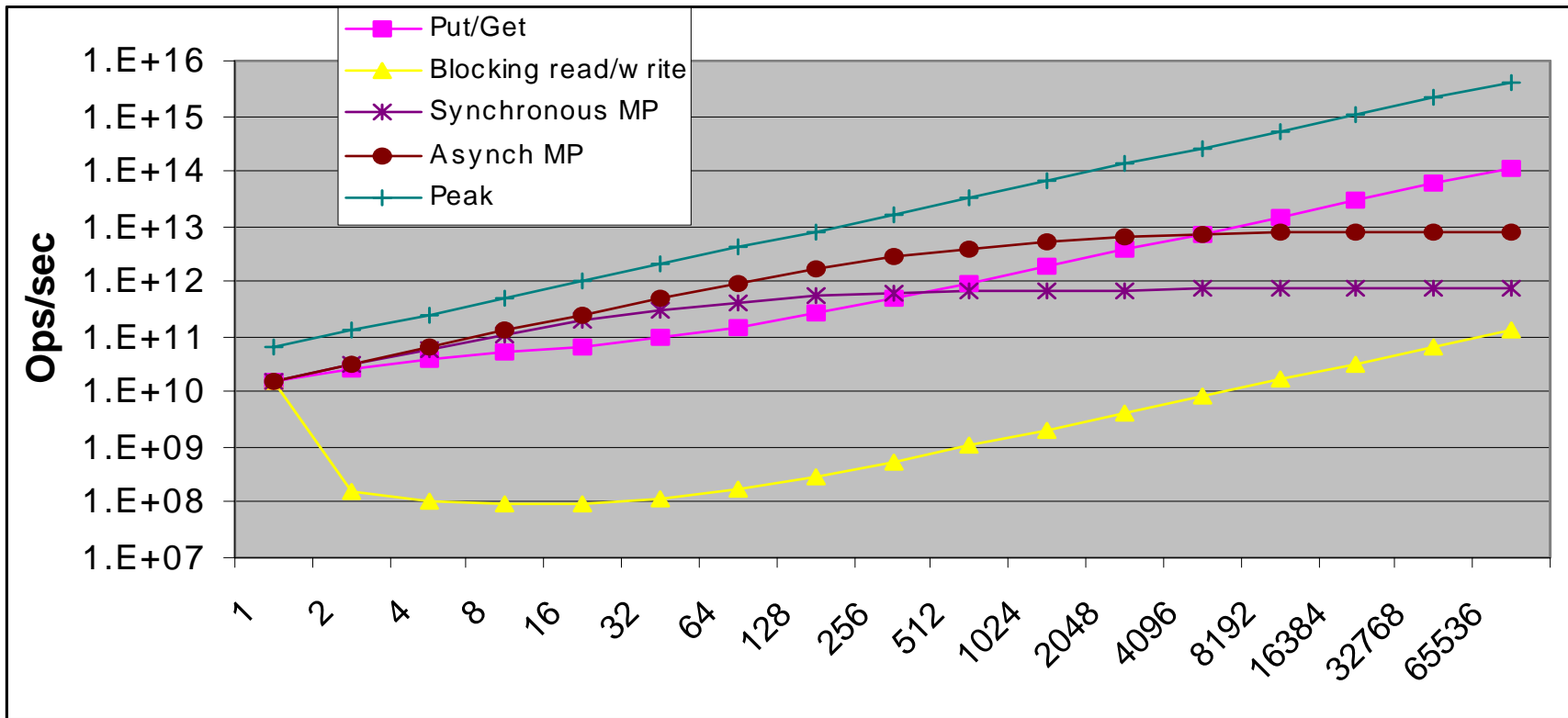


Scaling Applications



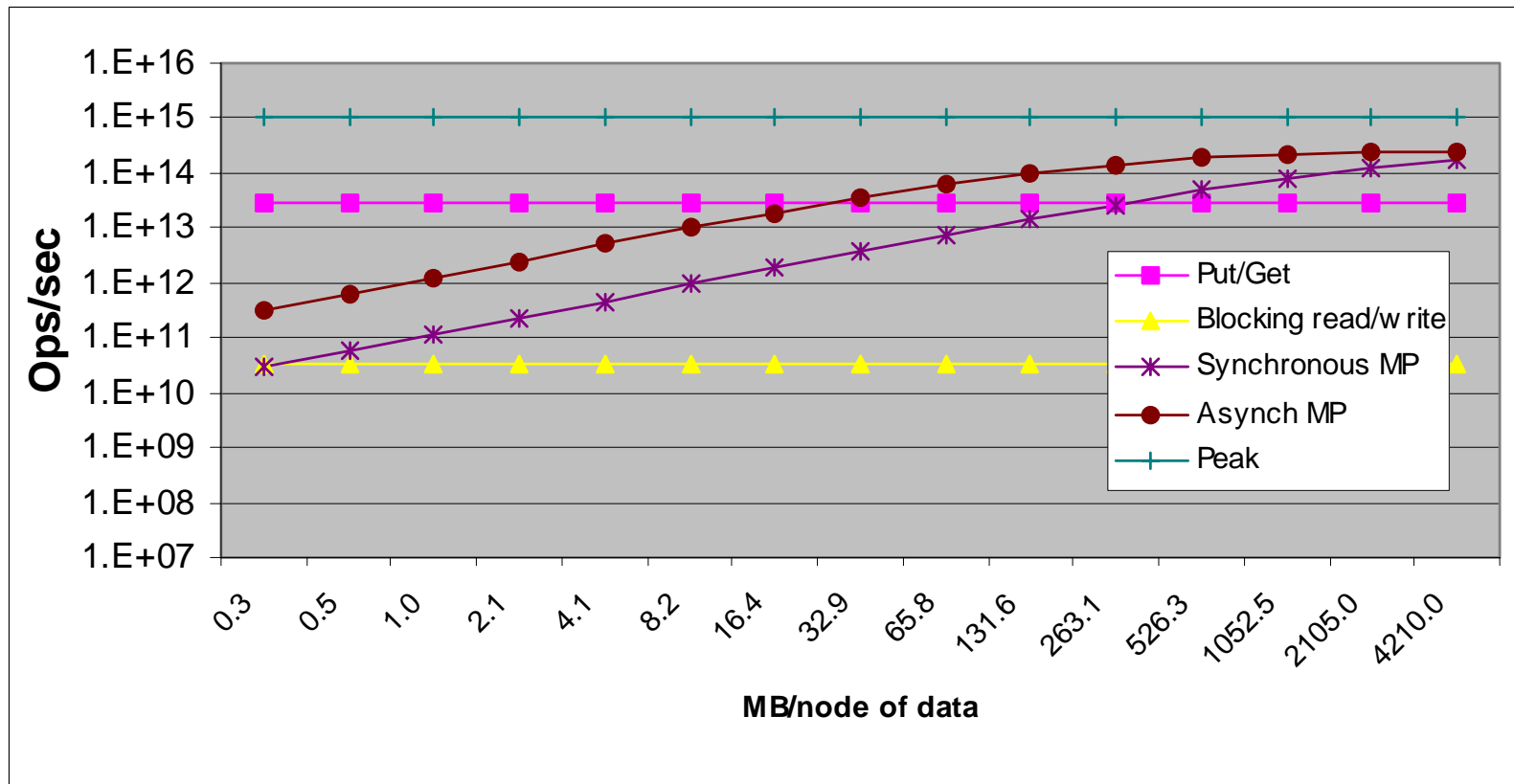
- **Machine Parameters**
 - **Floating point performance**
 - Application dependent, not theoretical peak
 - **Amount of memory per processor**
 - Use 1/10th for algorithm data
 - **Communication Overhead**
 - Time processor is busy sending a message
 - Cannot be overlapped
 - **Communication Latency**
 - Time across the network (can be overlapped)
 - **Communication Bandwidth**
 - Single node and bisection
- **Back-of-the envelope calculations !**

Running Sparse MVM on a Pflop



- $1 \text{ GHz} * 8 \text{ pipes} * 8 \text{ ALUs/Pipe} = 64 \text{ GFLOPS/node peak}$
- 8 Address generators limit performance to 16 Gflops
- 500ns latency, 1 cycle put/get overhead, 100 cycle MP overhead
- Programmability differences too: packing vs. global address space

Effect of Memory Size



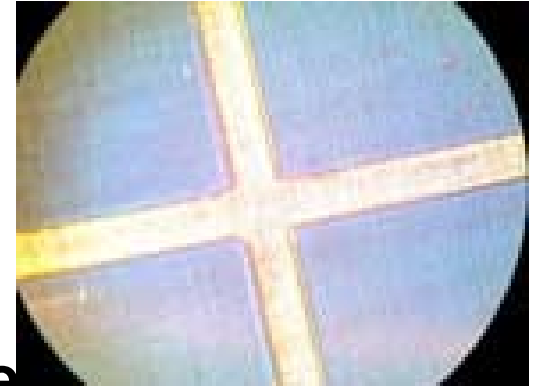
- Low overhead is important for
 - Small memory nodes or smaller problem sizes
 - Programmability

Parallel Applications in Titanium



- **Genome Application**
- **Heart simulation**
- **AMR elliptic and hyperbolic solvers**
- **Scalable Poisson for infinite domains**
- **Genome application**
- **Several smaller benchmarks: EM3D, MatMul, LU, FFT, Join**

MOOSE Application

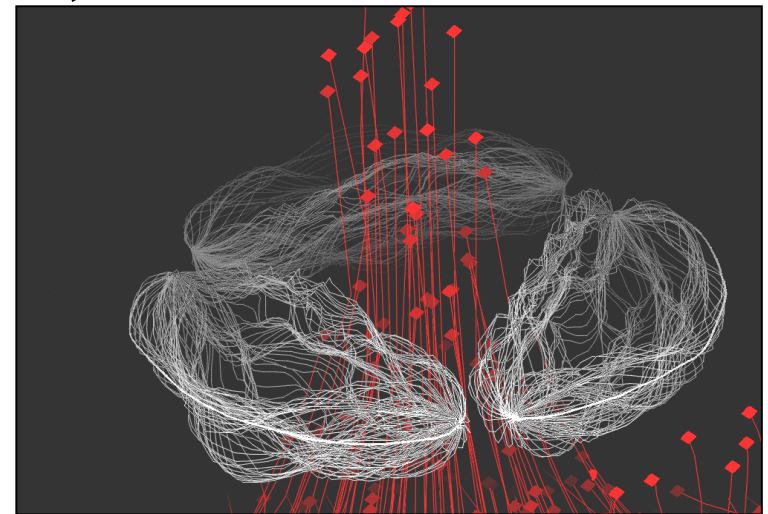


- **Problem: Microarray construction**
 - Used for genome experiments
 - Possible medical applications long-term
- **Microarray Optimal Oligo Selection Engine (MOOSE)**
 - A parallel engine for selecting the best oligonucleotide sequences for genetic microarray testing
 - Uses dynamic load balancing within Titanium

Heart Simulation



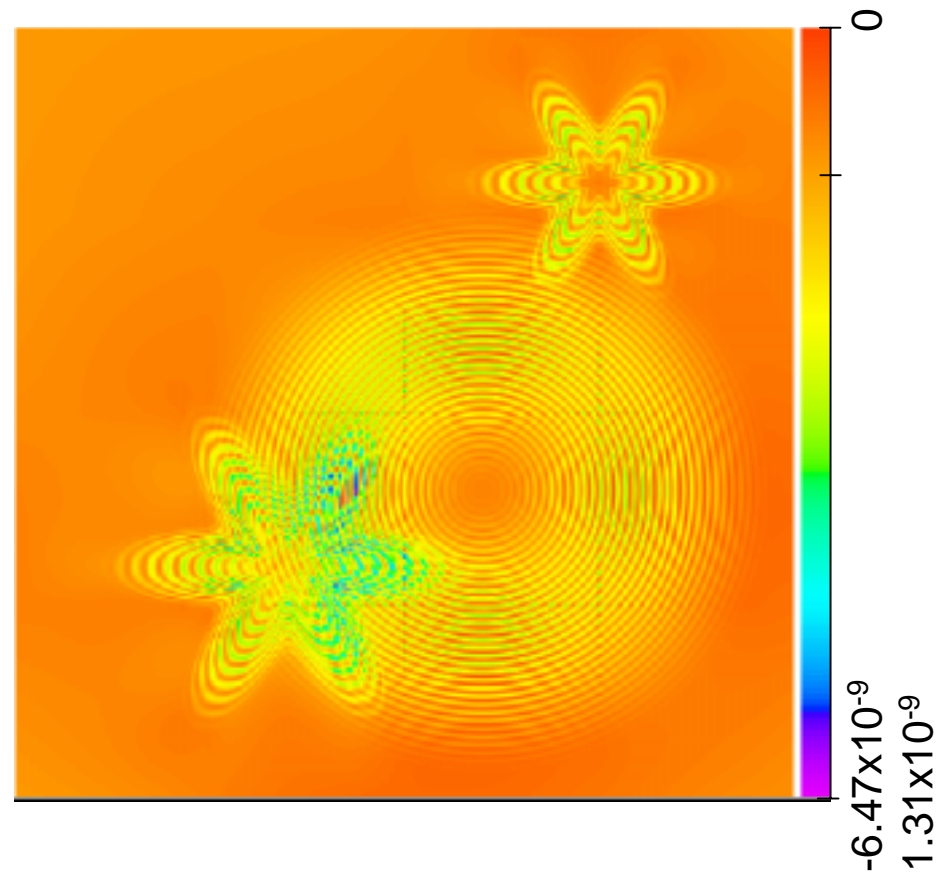
- **Problem: compute blood flow in the heart**
 - **Model as elastic structure in incompressible fluid.**
 - “Immersed Boundary Method” [Peskin and McQueen]
 - Particle/Mesh method stress communication performance
 - 20 years of development in model
 - **Many other applications: blood clotting, inner ear, insect flight, embryo growth,...**
- **Can be used for design of prosthetics**
 - **Artificial heart valves**
 - **Cochlear implants**



Scalable Poisson Solver



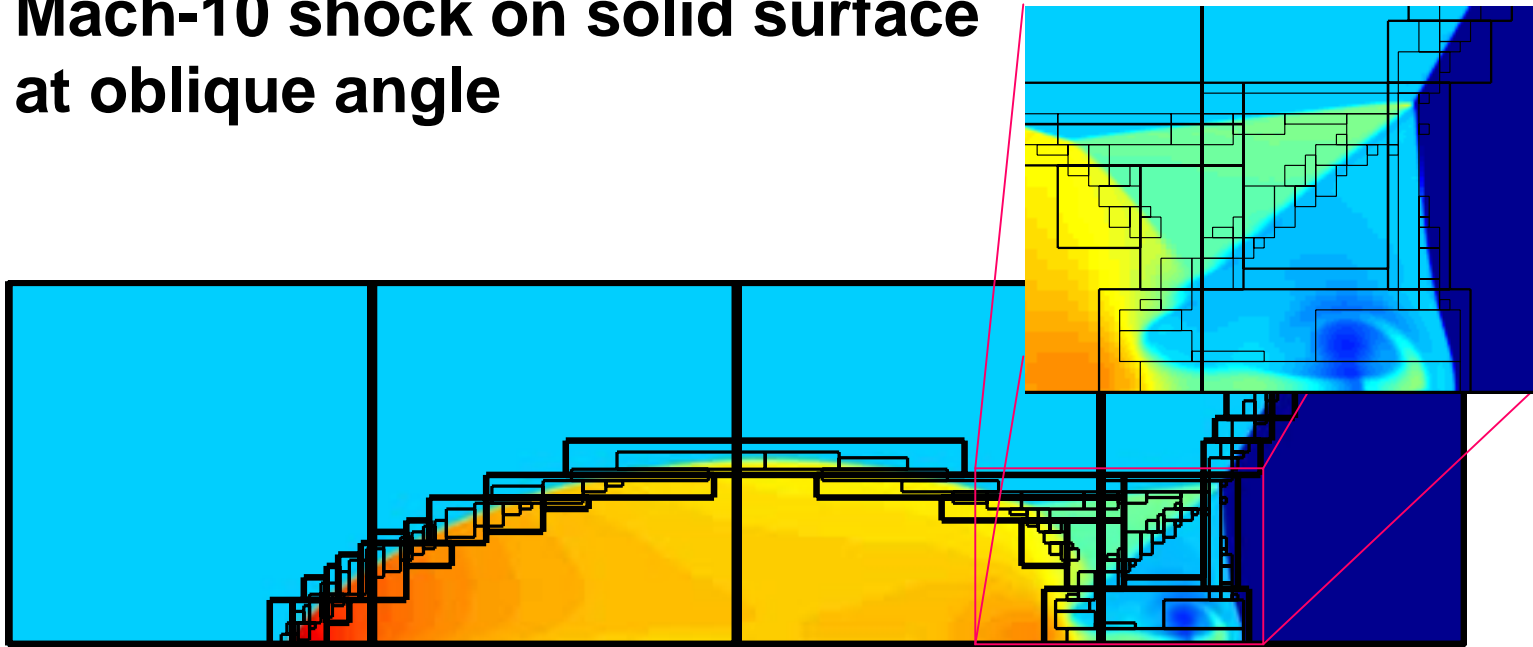
- **MLC for Finite-Differences by Balls and Colella**
- **Poisson equation with infinite boundaries**
 - arise in astrophysics, some biological systems, etc.
- **Method is scalable**
 - Low communication
- **Performance on**
 - SP2 (shown) and t3e
 - scaled speedups
 - nearly ideal (flat)
- **Currently 2D and non-adaptive**
- **Point charge example shown**
 - Rings & star charges
 - Relative error shown



AMR Gas Dynamics



- Developed by McCorquodale and Colella
- 2D Example (3D supported)
 - Mach-10 shock on solid surface at oblique angle



- Future: Self-gravitating gas dynamics package

UPC Application Investigations



- **Pyramid**
 - 3D Mesh generation [Shewchuk]
 - 2D version (triangle) critical in Quake project
 - Written in C, challenge to parallelize
- **SuperLU**
 - Sparse direct solver [Li, Demmel]
 - Written in C+MPI or threads
 - UPC may enable new algorithmic techniques
- **N-Body simulation**
 - “Simulating the Universe”

Summary



- **UPC Killer App should**
 - **Leverage programmability: hard in MPI**
 - **Use fine-grained, irregular, asynchronous communication**
- **Libraries**
 - **Must allow for interface to libraries**
 - **MPI libraries, multithreaded libraries, serial libraries**
- **Compilation needs**
 - **High performance on at least one machine**
 - **Portability across many machines**