

What is High Performance Computing? (and what does it have to do with you?)

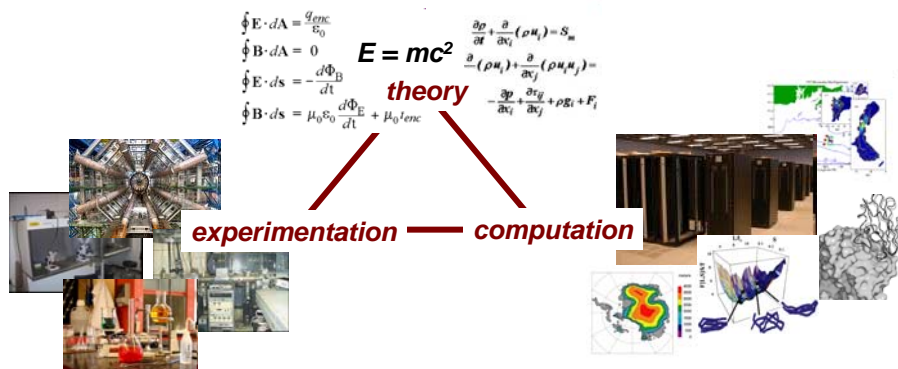
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Department of Computer Science
 Exec. Assoc. Dean, College of Natural Sciences
 Faculty Advisor for Science and Engineering, VCRE



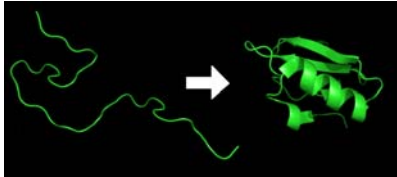
What is HPC?

- using large clusters of computers, or special-purpose "supercomputers" in computing applications that are too large or would take too long for "traditional" computing
- "third leg" of science, engineering inquiry



HPC application: protein folding

a protein begins as a long sequence of amino acids.....



.... which then **fold**s into a characteristic 3D functional structure for that protein

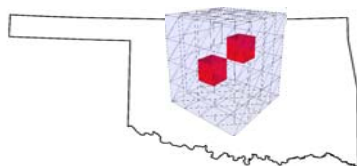
animation available at <http://www.youtube.com/watch?v=AlfvWESPyZY>

Proteins, made of chains of amino acids, carry out most cell functions, once folded into the proper structure. The movie starts with the final crystal structure of the villin protein (colors blue, white, red show different sequences in the protein), and then depicts how villin folds into its final structure over six microseconds.

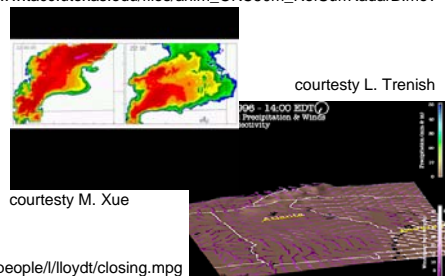
- ❑ understanding protein folding key to understanding:
 - ❖ **disease**: mis-folding linked to Alzheimer's, mad cow, others..
 - ❖ **drug design**: protein flexibility
- ❑ protein folding takes microseconds in vivo, but 100's CPU days to simulate: HPC

HPC application: numerical weather prediction

- ❑ computer simulation of weather/atmosphere evolution over time
- ❑ divide atmosphere into 3D grid, detailed simulation within each small (e.g., 10m³), gridpoint, couple with neighbors
- ❑ CASA: collaborative adaptive sensing of the atmosphere: UMass-led NSF Engineering Research Center



Animation available at http://www.tacc.utexas.edu/files/anim_OKC50m_RefSurfRadarB.mov



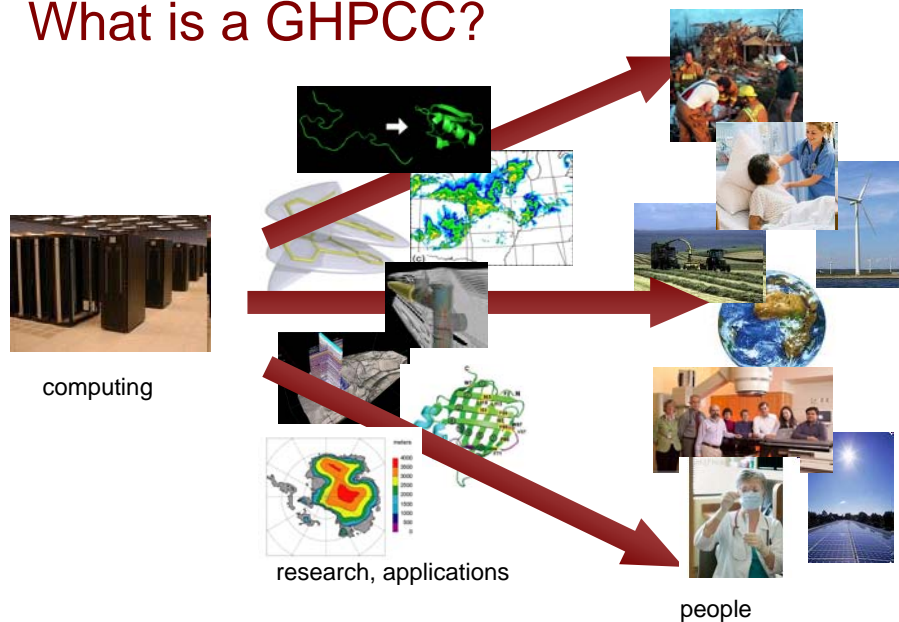
courtesy M. Xue

Animation available at <http://www.research.ibm.com/people/lloyd/closing.mpg>

Many (many!) other HPC application areas

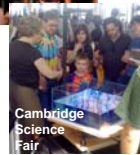
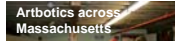
- ❑ **energy:** fuel cells, underground oil/gas location, flow
- ❑ **materials:** high-temperature superconductors, efficient catalysts
- ❑ **astronomy:** origins of the universe
- ❑ **physics:** low-temperature physics, high-energy physics (LHC)
- ❑ **finance:** financial modeling, trading analytics
- ❑ **environmental modeling:** earth, atmosphere, water
- ❑ **industry product design:** modeling versus physical prototyping, optimization
- ❑ **industry services:** complex data-driven decision-making, risk analysis, supply chain optimization, optimized routing

What is a GHPCC?



What is a GHPCC?

Not just this.....



this.....

**Education
and
Outreach**



UMass Amherst: state leadership in IT education

CITI: Commonwealth IT Initiative

- strengthening, modernizing, expanding IT education in *all segments* of public higher ed
 - ❖ building IT fluent workforce
 - ❖ culture of collaboration
- funded since 2000: BHE, foundations, industry, state
- programmatic:
 - ❖ IT across the curriculum
 - ❖ faculty development
 - ❖ curriculum enhancement



FOR THE GOOD Betty Medina Lichtenstein explains her needs to a University of Massachusetts class: from left, Jason De Faria, Prof. Carol Soules, Ryan Roy, Mankin Yuen and Erica Sawyer, a graduate assistant. *The New York Times* | 12/29/09

Betty Medina Lichtenstein of Enlace de Familias, Holyoke, working with UMass students/faculty on IT capstone course

UMass Amherst: state leadership in IT education

CAITE: Commonwealth Alliance for IT Education

Addressing under-representation in IT education and workforce, focusing on women and minorities in groups that are under-represented in the MA innovation economy.

- ❑ funded by \$4.1M NSF Broadening Participation in Computing grants
- ❑ focus on community colleges
- ❑ *outreach*: college/career fairs, campus visits, computing camps, IT internships
- ❑ *pathways*: intro courses, transfer agreements, peer mentoring, advising
- ❑ led by Rick Adrion, UMass/CS

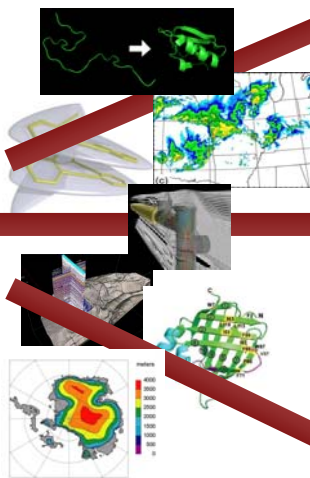


caite.cs.umass.edu

What is a GHPCC?



Not this!



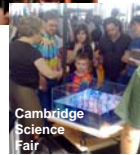
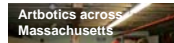
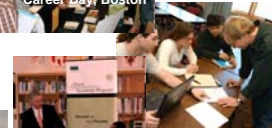
..... this!



.... and this!

What is a GHPCC?

Not just this.....



this.....

**Education
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Outreach**



Backup slides

What is the “G” in GHPCC?

Green energy sources

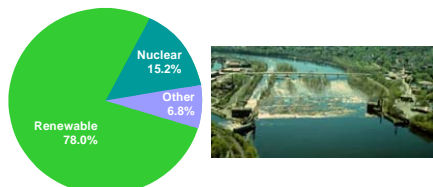


Figure 1: HG&E 2008 Energy Sources (2008)

Green facility operations

- ❑ state-of-the-art efficiency
- ❑ federated computing

Green computational science and engineering

- ❑ energy sciences
- ❑ environmental sciences
- ❑ green computing