MADNESS

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ORNL

CScADS workshop: Leadership-class Machines, Petascale Applications and Performance Strategies

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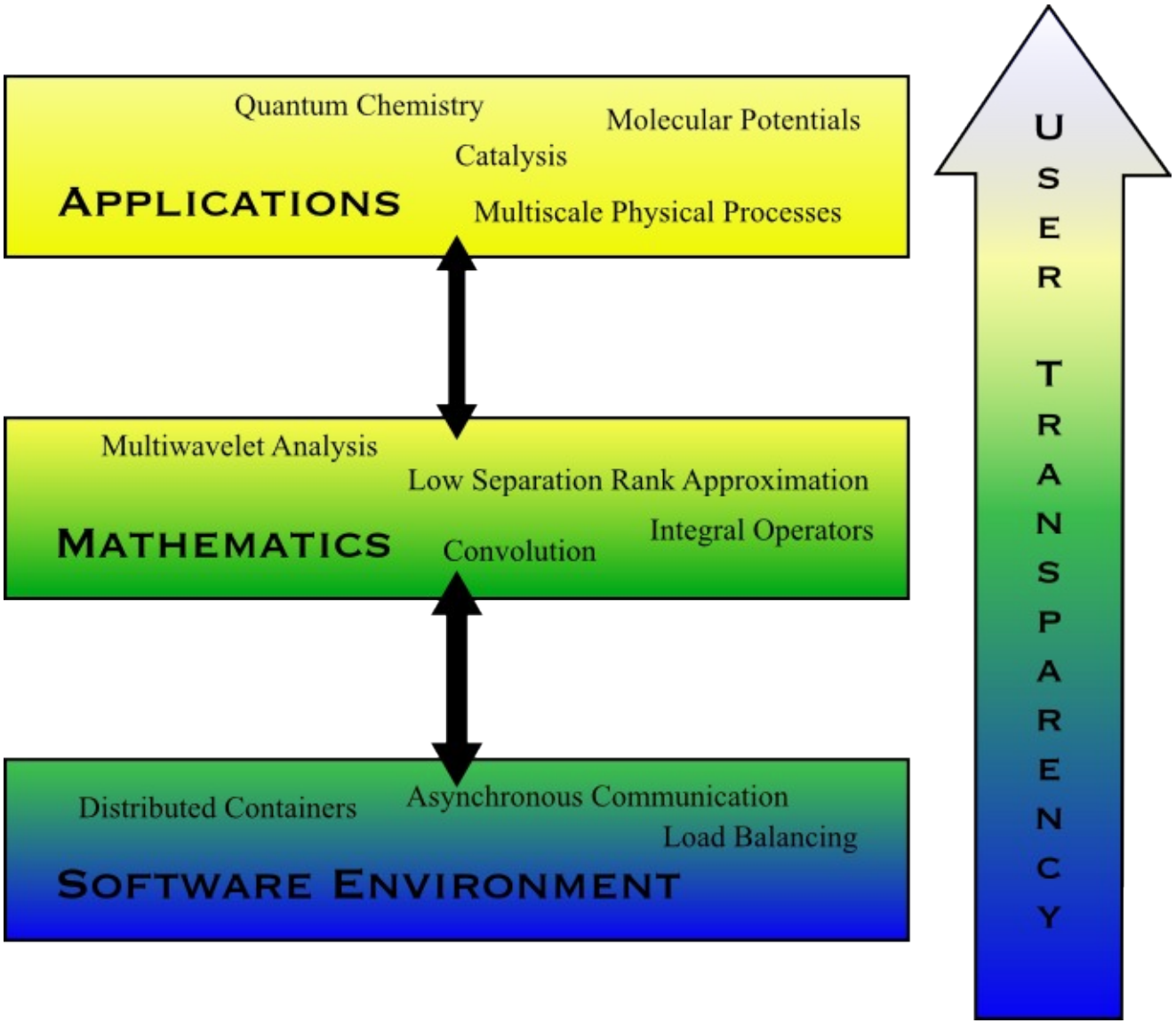
I. MADNESS

- ***M***ultiresolution ***Ad***aptive ***N***umerical ***E***nvironment for ***S***cientific ***S***imulation
- "Environment for prototyping and developing scientific applications using multiresolution analysis and low separation rank methods"
- Project Developers include George Fann, Robert Harrison, Gregory Beylkin, and Rebecca Hartman-Baker

MADNESS

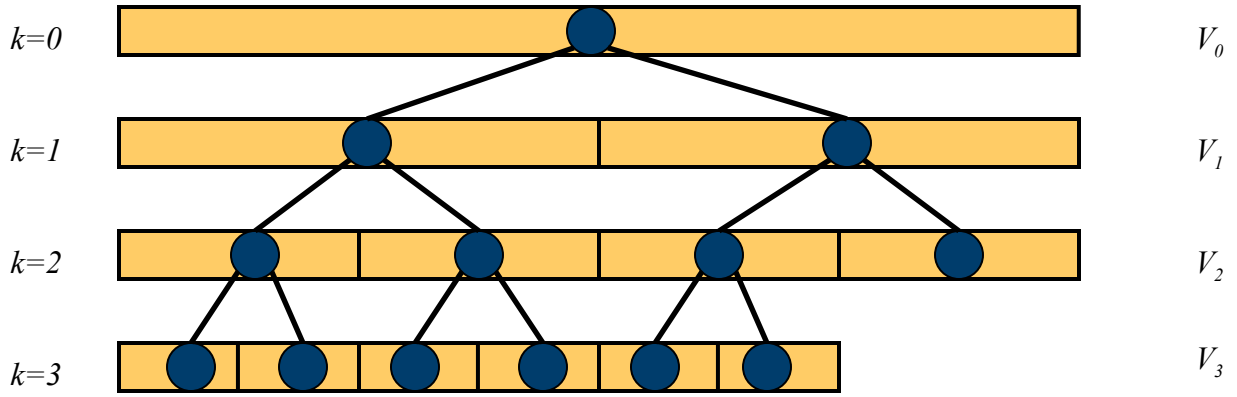

Quantum Chemistry
Molecular Potentials
Catalysis
APPLICATIONS
Multiscale Physical Processes
Multiwavelet Analysis
Low Separation Rank Approximation
MATHEMATICS
Integral Operators
Convolution
Distributed Containers
Asynchronous Communication
Load Balancing
SOFTWARE ENVIRONMENT
USER TRANSPARENCY

Computing Goals

- Run on leadership supercomputers; e.g., ORNL's Jaguar Cray XT5, Argonne's BlueGene/P, more advanced future systems
- Compute using $O(10^3–10^{5)}$ processors
- Solve problems resulting in trees with millions or billions of nodes

Representing a Function

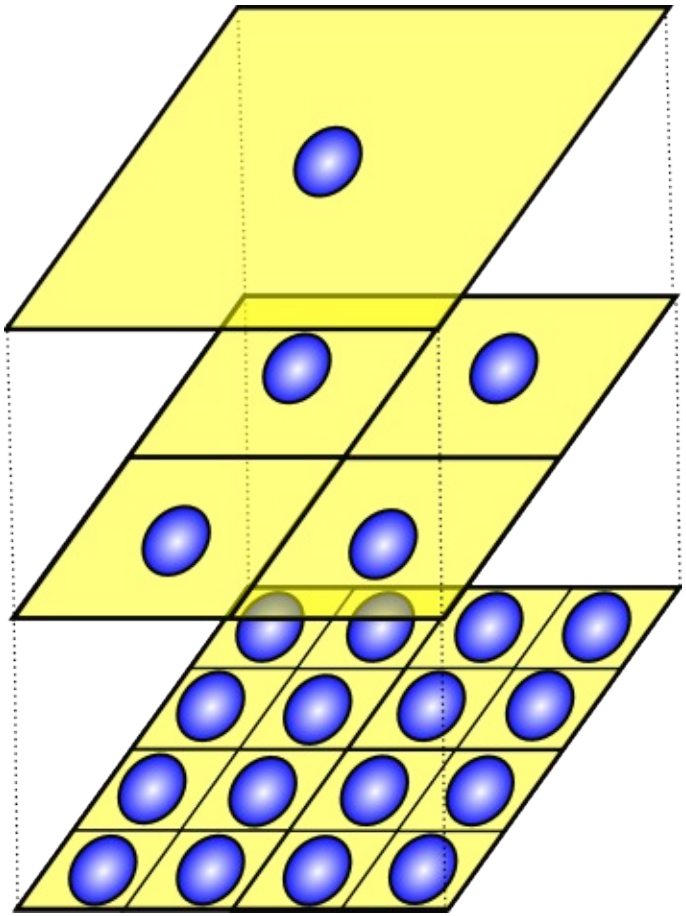
- In multiresolution analysis, represent function in scaling function space: a chain of embedded, closed subspaces
- Telescoping subspaces translate into tree form



- Adaptive refinement and truncation of coefficients means not all intervals may be subdivided

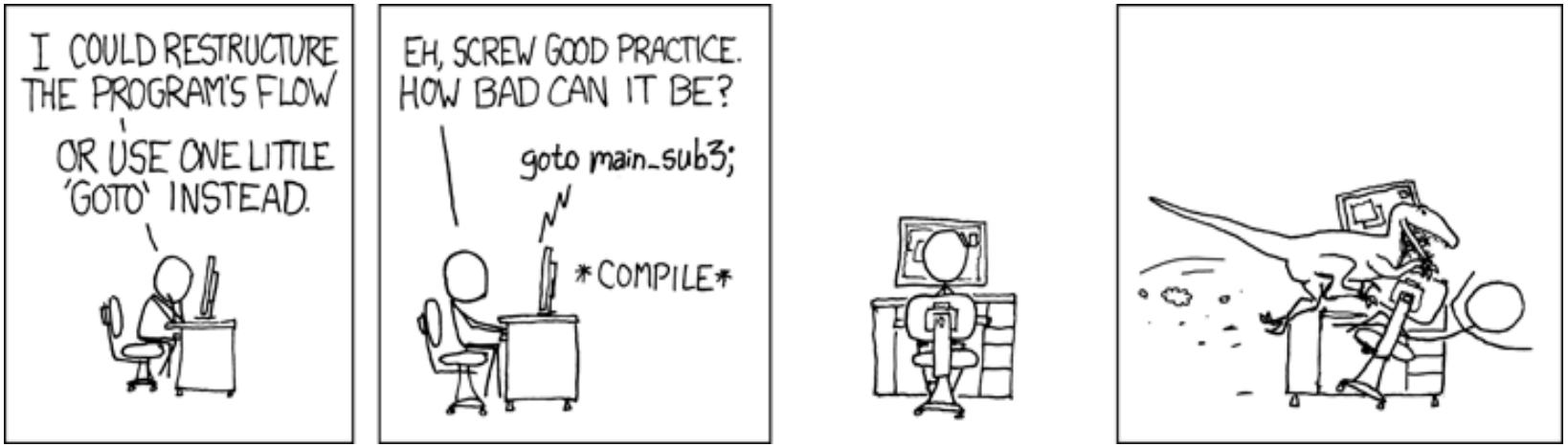
Representing a Function

- Same form for multiple dimensions
- Trees
  - Result of adaptive refinement of spatial domain
    - 2-D: quadtrees
    - 3-D: octrees
  - $O(10^6)$–$O(10^9)$ nodes in trees derived from target problems



Implementation of MADNESS

- Original proof-of-concept was written in Python
- New MADNESS written in C++
- Object-oriented design
- User transparency

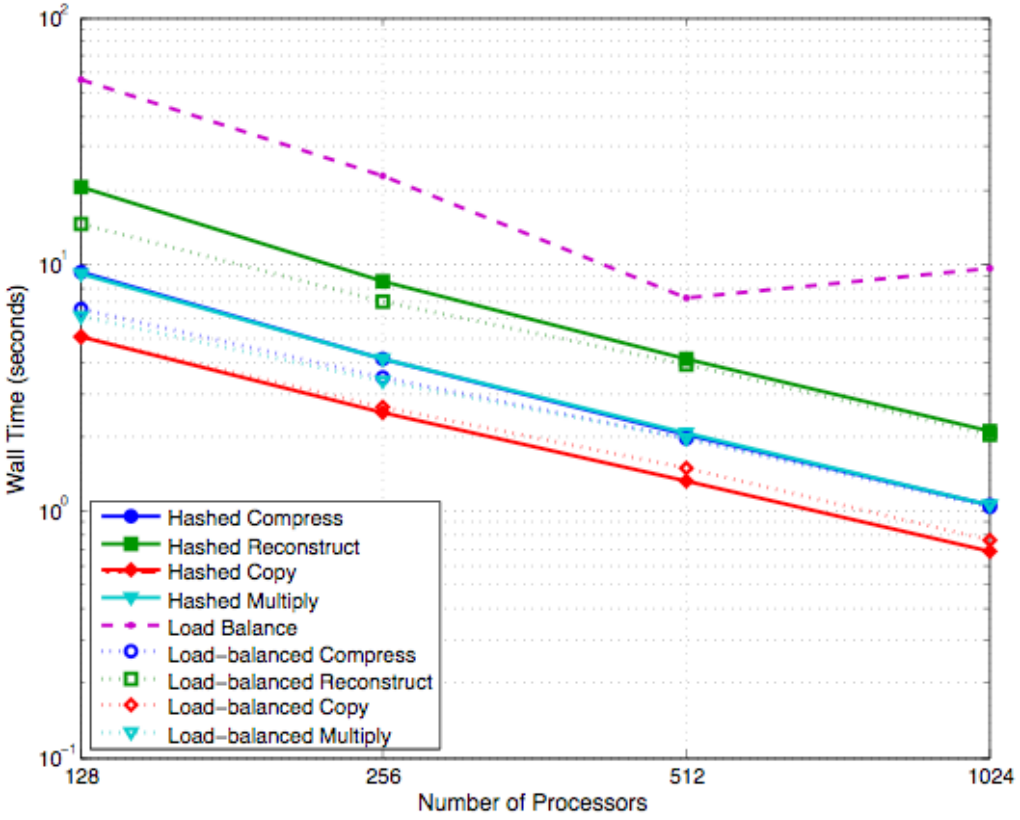


from http://xkcd.com/c292.html

Synthetic Test Problem

(work by Hartman-Baker, et al.)

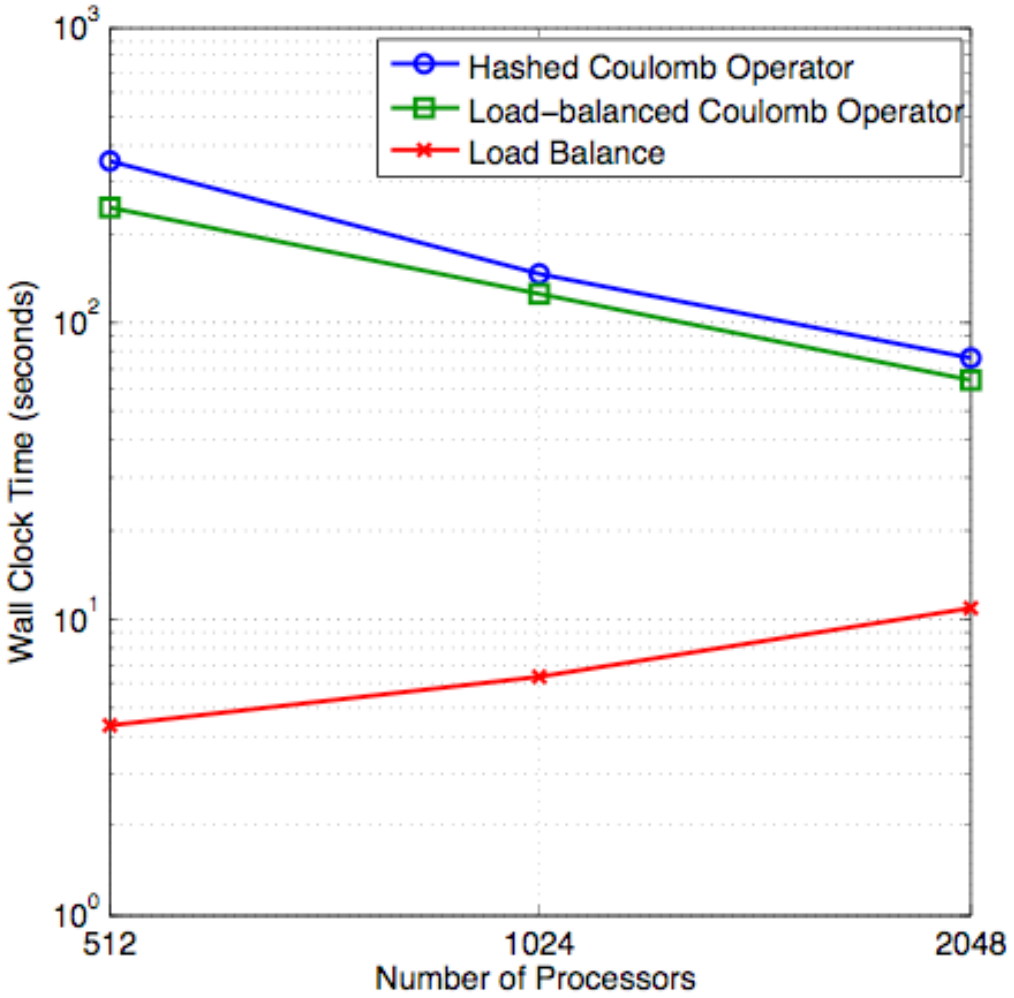
- Sum of Gaussians, with accuracy threshold 10^{-12}
- Approximate using multiwavelet degree $k = 5$
  - 2.06×10^6 nodes
  - 2.25×10^8 coefficients
- Benefit of load balancing declines as amount of work per processor shrinks



Application Problem

(work by Hartman-Baker, et al.)

- Compute Coulomb potential of lattice of 4096 copper atoms
- Rising cost of load balancing is indictment of hashed distribution
- Act of load balancing comparable in cost to simple mathematical operation (e.g. projection)



More on MADNESS

- URLs
  - MADNESS: http://www.csm.ornl.gov/ccsg/html/projects/madness.html
  - MADNESS code repository: http://code.google.com/p/m-a-d-n-e-s-s/
  - SCIDAC project webpage: http://www.csm.ornl.gov/~hqi/scidac/
- Papers (Math)
  - B. Alpert, "A class of bases in L2 for the sparse representation of integral operators," SIAM J. Math. Anal. 24, pp. 246–262, 1993.
  - B. Alpert, G. Beylkin, D. Gines, and L. Vozovoi, "Adaptive solution of Partial Differential Equations in multiwavelet bases," *J. Comp Phys 182*, pp. 149–190, 2002.
  - G. Fann, G. Beylkin, R.J. Harrison, and K.E. Jordan, "Singular operators in multiwavelet bases," *IBM J. Res. & Dev. 48(2),* pp. 161–171, 2004.
  - R.J. Hartman-Baker, R.J. Harrison, and G.I. Fann, "Load Distribution in MADNESS," *in preparation.*

Acknowledgments

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