

World Community Grid Managing our research projects







World Community Grid's Mission

World Community Grid's mission is to create the world's largest public computing grid to tackle projects that benefit humanity.

- Engage volunteers who want to contribute their computers to humanitarian research projects
- Provide free computing power to research projects whose findings may provide a humanitarian benefit
- Use the depth and breadth of IBM to build the power and capability of the grid
- Achieve results that are openly shared







Active Research@World Community Grid

- Computing for Clean Water, Tsinghua University
- The Clean Energy Project, Harvard University
- Discovering Dengue Drugs Together, University of Texas Medical Branch
- Help Cure Muscular Dystrophy, Université Pierre et Marie Curie
- Help Fight Childhood Cancer, Chiba Cancer Center Research Institute
- Help Conquer Cancer, Ontario Cancer Institute
- Human Proteome Folding, New York University
- FightAIDS@Home, The Scripps Research Institute







Completed Research@World Community Grid

- Influenza Antiviral Drug Search, University of Texas Medical Branch (25 million hours donated)
- Nutritious Rice for the World, University of Washington (225 million hours donated)
- AfricanClimate@Home, University of Cape Town (300 thousand hours donated)
- Genome Comparison, Oswaldo Cruz Institute (33 million hours donated)
- Help Defeat Cancer, The Cancer Institute of New Jersey (26 million hours donated)







How Projects are Selected

- Easy to submit a proposal. See http://www.worldcommunitygrid.org/research/viewSubmitAProposal.do
- Requirements:
 - Focused on solving problems to benefit humanity;
 - Conducted by public or nonprofit organizations;
 - Contributed to the public domain; and
 - Accelerated by grid computing technology.



Proposals are reviewed by subject matter experts from both within and outside of IBM





On-Boarding – Application Modifications

- Detailed meetings with researchers to understand how application works
- Time spent 'up-sizing' compute power that will be available for the research
- Security review of code
- Modify code to support checkpointing and interface with the BOINC API
- Development of graphics visualizing the work in process
- Develop Validator
- Develop Assimilator
- Alpha Testing
- Beta Testing







On-Boarding – Website Preparations

- Develop home page logo and content
- Develop detailed descriptions of project
- Develop member badges
- Develop slide show images (for simple user interface)

<u>Bearcat</u> Veteran Cruncher	Re: Welcome to the Computing for Clean Water project!
	More than happy to crunch for a worthy cause.
	Crunching for humanity!
USA	
Joined: Jan 6, 2007	
Post Count: 566	
Status: Offline	
Project Badges:	
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On-Boarding – Publicity

- Meetings to discuss launch press releases
- Timing and content coordinated between IBM and the press office of the organization whose project is launching
- Promotion Video YouTube
- Email messages sent to members
- Home page announcement
- News and Updates messages (website, RSS)
- Facebook
- Twitter





On-Going

- Data transfer between researchers and World Community Grid
- Workunit preparation and result packaging
- Monitoring application for errors
- Forum support
- User support





Project Completion

- Notify members and mark project as completed
- Maintain communication with researchers
- Notify members of papers published
- Help ensure that the data is placed online
- Celebrate!





Volunteered Computing Power

- In the past 30 days:
 - Over 90,000 volunteers have contributed computer time
 - Over 180,000 computers have contributed computer time
 - Over 75,000,000 hours of computing time have been returned
- Yesterday
 - Over 54,000 volunteers contributed computer time
 - Over 103,000 computers contributed computer time
 - Over 2,800,000 hours of computing time





Results – Papers

- 17 peer-reviewed papers published based on the research run on World Community Grid
- Genome Comparison 1
- Help Conquer Cancer 3
- Help Cure Muscular Dystrophy 3
- Help Defeat Cancer 3
- Discovering Dengue Drugs Together 1
- Human Proteome Folding 5
- FightAIDS@Home 1

Detailed list of papers available in appendix





Results – Accomplishments

- Help Defeat Cancer Based on the work down on World Community Grid, the research team was awarded NIH funding to establish a gold standard reference library of imaged specimens and software. Initial results show that this automated method produces equal to those of the best pathologists, with more graduated scoring and potentially faster throughput. This should permit earlier identification of potential cancers earlier while they are more curable. The NIH funded project, scheduled for completion in 10/2011, has already deployed the software at three cancer centers with plans to make the imaging tools and reference library available to all major US cancer centers.
- FightAIDS@Home Identified seven promising hits from a large compound library that in follow-up laboratory experiments appeared to be effective inhibitors against a drug-resistant strain of HIV protease, but subsequent laboratory tests indicated that they likely would have toxic side effects. However, additional screenings of other compound libraries have identified promising leads which potentially disable the HIV protease in a new and different manner than prior inhibitors. This new way of inhibiting the HIV protease might prove to be a significant breakthrough and advance over conventional inhibitors, which are defeated by the frequent mutations of the AIDS virus.
- Human Proteome Folding Have predicted the structures of proteins and added this information to public data bases which are used by scientists around the world.
- Genome Comparison Computed a complete pair-wise comparison between all currently sequenced genes to obtain similarity indices. This data now resides in a public data base that is used by scientists around the world.
- Influenza Antiviral Drug Search Screened 3 million molecules for their possible interaction with certain proteins (e.g., neuraminidase) required for the influenza viruses to replicate, with a focus on drug resistant strains. Pending a second phase focusing on the top 2,000 candidates.
- Discovering Dengue Drugs Together Screened 3 million compounds against 15 target enzymes from dengue, hepatitis C, and West Nile viruses in the Flaviviridae family to identify promising drug leads to combat these diseases. A second phase is in progress focusing on refining the top 2,000 candidates.





Questions?





Appendix – Published Papers

- Thomas Dan Otto, Marcos Catanho, Cristian Tristão, Márcia Bezerra, Renan Mathias Fernandes, Guilherme Steinberger Elias, Alexandre Capeletto Scaglia, Bill Bovermann, Viktors Berstis, Sergio Lifschitz, Antonio Basílio de Miranda, and Wim Degrave. ProteinWorldDB: querying radical pairwise alignments among protein sets from complete genomes. Bioinformatics Advance Access published on March 1, 2010, DOI 10.1093/bioinformatics/btq011. Bioinformatics 26: 705-707. (Genome Comparison)
- Cumbaa CA, Jurisica I. Protein crystallization analysis on the World Community Grid. J Struct Funct Genomics. 2010 Mar;11(1):61-9. Epub 2010 Jan 14. (Help Conquer Cancer)
- Viktors Berstis, Raphaël Bolze, Frédéric Desprez and Kevin Reed. From Dedicated Grid to Volunteer Grid: Large Scale Execution of a Bioinformatics Application. Journal of Grid Computing. August, 2009. Volume 7, Number 4, 463-478, DOI: 10.1007/s10723-009-9130-7 (Help Cure Muscular Dystrophy)
- Yang L, Chen W, Meer P, Salaru G, Goodell LA, Berstis V, Foran DJ. Virtual microscopy and grid-enabled decision support for large-scale analysis of imaged pathology specimens. IEEE Trans Inf Technol Biomed. 2009 Jul; 13(4):636-44. Epub 2009 Apr 14. (Help Defeat Cancer)
- S. M. Tomlinson, R. D. Malmstrom and S. J. Watowich. New Approaches to Structure-Based Discovery of Dengue Protease Inhibitors. Infect Disord Drug Targets. 2009 Jun;9(3):327-43. (Discovering Dengue Drugs – Together)
- Yang L, Tuzel O, Chen W, Meer P, Salaru G, Goodell LA, Foran DJ. PathMiner: a Web-based tool for computer-assisted diagnostics in pathology. IEEE Trans Inf Technol Biomed. 2009 May;13(3):291-9. Epub 2009 Jan 20. (Help Defeat Cancer)
- Engelen S, Trojan LA, Sacquin-Mora S, Lavery R, Carbone A, Joint Evolutionary Trees: A Large-Scale Method To Predict Protein Interfaces Based on Sequence Sampling. PLoS Comput Biol 2009 5(1): e1000267. doi:10.1371/journal.pcbi.1000267 (Help Cure Muscular Dystrophy)
- Edward H. Snell, Angela M. Lauricella, Stephen A. Potter, Joseph R. Luft, Stacey M. Gulde, Robert J. Collins, Geoff Franks, Michael G. Malkowski, Christian Cumbaa, Igor Jurisica, and George T. DeTitta. Establishing a training set through the visual analysis of crystallization trials. Part II: crystal examples. Acta Crystallogr D Biol Crystallogr. 2008 November 1; 64(Pt 11): 1131–1137. Published online 2008 October 18. doi: 10.1107/S0907444908028059. (Help Conquer Cancer)
- Edward H. Snell, Joseph R. Luft, Stephen A. Potter, Angela M. Lauricella, Stacey M. Gulde, Michael G. Malkowski, Mary Koszelak-Rosenblum, Meriem I. Said, Jennifer L. Smith, Christina K. Veatch, Robert J. Collins, Geoff Franks, Max Thayer, Christian Cumbaa, Igor Jurisica, and George T. DeTitta. Establishing a training set through the visual analysis of crystallization trials. Part I: ~150 000 images. Acta Crystallogr D Biol Crystallogr. 2008 November 1; 64(Pt 11): 1123–1130. doi: 10.1107/S0907444908028047. (Help Conquer Cancer)
- DiPaola, R. S., Dvorzhinski, D., Thalasila, A., Garikapaty, V., Doram, D., May, M., Bray, K., Mathew, R., Beaudoin, B., Karp, C., Stein, M., Foran, D. J. and White, E. (2008), Therapeutic starvation and autophagy in prostate cancer: A new paradigm for targeting metabolism in cancer therapy. The Prostate, 68: 1743–1752. doi: 10.1002/pros.20837 (Help Defeat Cancer)
- Mike Boxem, Zoltan Maliga, Niels Klitgord, Na Li, Irma Lemmens, Miyeko Mana, Lorenzo de Lichtervelde, Joram D. Mul, Diederik van de Peut, Maxime Devos, Nicolas Simonis, Muhammed A. Yildirim, Murat Cokol, Huey-Ling Kao, Anne-Sophie de Smet, Haidong Wang, Anne-Lore Schlaitz, Tong Hao, Stuart Milstein, Changyu Fan, Mike Tipsword, Kevin Drew, Matilde Galli, Kahn Rhrissorrakrai, David Drechsel, Daphne Koller, Frederick P. Roth, Lilia M. Iakoucheva, A. Keith Dunker, Richard Bonneau, Kristin C. Gunsalus, David E. Hill, Fabio Piano, Jan Tavernier, Sander van den Heuvel, Anthony A. Hyman, Marc Vidal, *A Protein Domain-Based Interactome Network for C. elegans Early Embryogenesis*, Cell, Volume 134, Issue 3, 8 August 2008, Pages 534-545, ISSN 0092-8674, DOI: 10.1016/j.cell.2008.07.009. (Human Proteome Folding)
- Sophie Sacquin-Mora, Alessandra Carbone, Richard Lavery, Identification of Protein Interaction Partners and Protein-Protein Interaction Sites, Journal of Molecular Biology, Volume 382, Issue 5, 24 October 2008, Pages 1276-1289, ISSN 0022-2836, DOI: 10.1016/j.jmb.2008.08.002. (Help Cure Muscular Dystrophy)
- Bonneau, Richard; Facciotti, Marc T.; Reiss, David J.; Schmid, Amy K.; Pan, Min; Kaur, Amardeep; Thorsson, Vesteinn; Shannon, Paul; Johnson, Michael H.; Bare, J. Christopher; Longabaugh, William; Vuthoori, Madhavi; Whitehead, Kenia; Madar, Aviv; Suzuki, Lena; Mori, Tetsuya; Chang, Dong-Eun; DiRuggiero, Jocelyne; Johnson, Carl H.; Hood, Leroy; Baliga, Nitin S. A Predictive Model for Transcriptional Control of Physiology in a Free Living Cell. doi:10.1016/j.cell.2007.10.053 (volume 131 issue 7 pp.1354 - 1365) (Human Proteome Folding)
- Max W. Chang, William Lindstrom, Arthur J. Olson, and, Richard K. Belew. Analysis of HIV Wild-Type and Mutant Structures via in Silico Docking against Diverse Ligand Libraries. Journal of Chemical Information and Modeling 2007 47 (3), 1258-1262 (FightAIDS@Home)
- Lars Malmström, Michael Riffle, Charlie E. M. Strauss, Dylan Chivian, Trisha N. Davis, Richard Bonneau, David Baker. Superfamily Assignments for the Yeast Proteome through Integration of Structure Prediction with the Gene Ontology. 2007 PLoS Biol 5(4): e76. doi:10.1371/journal.pbio.0050076 (Human Proteome Folding)
- Erica Andersen-Nissen, Kelly D. Smith, Richard Bonneau, Roland K. Strong, and Alan Aderem. A conserved surface on Toll-like receptor 5 recognizes bacterial flagellin. Published February 5, 2007 // JEM vol. 204 no. 2393-403. The Rockefeller University Press, doi: 10.1084/jem.20061400. (Human Proteome Folding)
- Iliana Avila-Campillo, Kevin Drew, John Lin, David J. Reiss and Richard Bonneau. BioNetBuilder: automatic integration of biological networks. Bioinformatics 2007 23(3):392-393;
 doi:10.1093/bioinformatics/btl604 (Human Proteome Folding)