



Engaging Researchers







IBM Values

Dedication to every client's success.

Innovation that matters — for our company and for the world.

Trust and personal responsibility in all relationships.



IBM's Corporate Citizenship & Corporate Affairs Strategy

- Demonstrate the positive potential of IT's contribution to social needs and development
- Leverage our capabilities (expertise, software and hardware) and embed within global programs
- Develop programmes with partners with deep expertise
- Deploy programmes with governments and partners with strong local knowledge
- Aim to strengthen the communities where we do business

Real change, not just spare change







What is World Community Grid?

- A public volunteer computing grid supported by IBM
- A free computing resource for research that is pursuing a humanitarian goal
- A long term home for volunteers who can participate in multiple research projects









- Launched in Nov '04
- Modeled on United Devices - Grid.org
- Runs on BOINC
- RFP for new projects





- Runs on Windows, Linux, and Mac devices
- May expand to run on GPU/Cuda and cell









Our Team...



One virtual team.....

- Project team (full time):
 - Chicago, Illinois, USA 2 people Website, BOINC, and Hosting Management
 - Austin, Texas, USA: 3 people Scientific Support, Project Enablement, Work Management
 - Atlanta, Georgia, USA: 2 people Administrative Support
 - Seattle, Washington, USA: 1 person Project Management
- New York, New York, USA: Executive Sponsorship
- Toronto, Canada: Hosting Environment
- Berkeley, California: The BOINC team
- Community Advisors: 6 volunteers from around the world
- Worldwide: IBM colleagues plus community relations people in every country.
- Worldwide: 400+ Partners potentially recruiting members and research projects.
- Worldwide: Researchers from non-profit organizations.







Facts.....

- Total Registered Members: Nearly 500,000
 - Adding an average of 1,500 members per week
- Total Registered Devices: Nearly 1.5 million
 - Adding an average of 5,000 devices per week
- Total Computer Run Time: Nearly 300,000 Years
 - Receiving an average of 2,000 years per week
 - Equates to about 340 Teraflops
- Total Research Results: 333 million
 - Equates to about 5 result transactions per second
- Volunteers from 200+ countries





Visit WorldCommunityGrid.org

- Joining
- Statistics
- Project information
- Help information FAQ's
- Forums
- Teams, challenges, badges
- Widget, RSS feed
- Partners
- Preferences
- Submitting proposals

Teams









Security

- Security is a top concern for World Community Grid to ensure the trust of our partners and individual volunteers.
- Agent initiates all communications
- Communications encrypted
- Public-private key authentication
- Secure hosting center
- Ongoing security audits
- Agent software certificate
- Device registration
- Security audits of executable code

We install the client on all IBM-owned workstations and encourage our employees to activate it!







World Community Grid assumes the burden of running the grid





Humanitarian research gets a free supercomputing boost



- Grid enabling research software
- Testing (Alpha & Beta)
- Formal Project Launches
- Receive researchers data
- Work unit Management
- Data Backups
- Send results to researchers
- Monitoring disk space
- Checking errant devices
- Problem work units
- Helping the scheduler
- Web site modifications
- Forum monitoring
- Support emails
- Soliciting new research
- System updates / upgrades
- Audits







What do the researchers do and what does World Community Grid do?

Applications









Typical Project

- Humanitarian project proposed which requires massive amounts of computing power to solve
- Project is reviewed but subject matter experts
- IBM team prepares the research code for running on World Community Grid
- Large computing problem is split into millions of smaller independent runs
- Servers send those work units to donor machines around the world
- The machines return their results after they have processed them
- Servers assemble pieces of the answers to produce the final results of the research project
- Results made available in the public domain









What research is being run on World Community Grid



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Help Fight Childhood Cancer Chiba Cancer Center

<u>The Clean Energy Project</u>
Department of Chemistry and Chemical Biology,

Help Cure Muscular Dystrophy Université Pierre et Marie Curie, AFM (French

 Influenza Antiviral Drug Search University of Texas Medical Branch, Galveston

Discovering Dengue Drugs - Together University of Texas Medical Branch, Galveston

Nutritious Rice for the World University of Washington

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Help Conquer Cancer Ontario Cancer Institute

Human Proteome Folding New York University

FightAIDS@Home The Scripps Research Institute

AfricanClimate@Home University of Cape Town

Genome Comparison Laboratório de Genômica - Funcional e

Help Defeat Cancer Cancer Institute of New Jersey







Influenza Antiviral Drug Search Project

- Launched May 2009
- Sponsored by Dr. Stan Watowich and his research team at The University of Texas Medical Branch (Galveston, Texas, USA)
- The mission of the Influenza Antiviral Drug Search project is to find new drugs that can stop the spread of an influenza infection in the body. The research will specifically address the influenza strains that have become drug resistant as well as new strains that are appearing.
- Identifying the chemical compounds that are the best candidates, will accelerate the efforts to develop treatments that would be useful in managing seasonal influenza outbreaks, and future influenza epidemics and even pandemics.
- One promising approach to combat these viruses and prevent them from causing disease is to develop new drugs that inhibit neuraminidase (N1, N2, etc), NS1 protein, hemagglutinin, and possibly other targets that influenza needs to spread in the body. Using the known chemical structures of these target molecules, the project will perform virtual chemistry experiments and determine which of millions of known compounds attach to these target molecules in a manner that can disable or inhibit them, thus potentially keeping the influenza virus from spreading in the body.









Help Cure Muscular Dystrophy Phase 1 and 2

- Phase 1: Sponsored by by the Association Francaise Contre Les Myopathies (Paris, France)
 - Launched December 2006 and completed June 2007.
 - Searched for binding sites between proteins, genes, their genetic variations, ligands (potential drugs) involved in neuromuscular diseases, with a particular focus on Muscular Dystrophy.
 - Conceptualized and confirmed a numerical methodology discriminating protein partners from non-interacting pairs of proteins (for a pool of protein pairs whose interaction was known).
- Phase 2: Sponsored by Decrypthon (a partnership of AFM/IBM/CNRS) and the Universite Pierre et Marie Curie.
 - Launched May 2009
 - This phase of the project will apply the numerical method on protein pairs whose interaction is unknown to discover new potential protein partners.
 - Contribution to this project will result in valuable information for biologists and physicians, and eventually will benefit all researchers working on genetic diseases, particularly, neuromuscular diseases.
 - This phase of the project will apply the methods validated and refined in Phase 1, to determine how all of over 2000 proteins, involved in neuromuscular diseases, interact with each other.









Help Fight Childhood Cancer

- Launched March 2009
- Sponsored by Chiba Cancer Center Research Institute and Chiba University
- The main goal of the project is to is to find drugs that can disable three particular proteins associated with neuroblastoma, one of the most frequently occurring solid tumors in children. Identifying these drugs could potentially make the disease much more curable when combined with chemotherapy treatment.
 - the project's researchers are using computational methods to identify new candidate drugs that have the right shape and chemical characteristics to block three proteins - TrkB, ALK and SCxx, which are expressed at high levels or abnormally mutated in aggressive neuroblastomas. If these proteins are disabled, scientists believe there should be a high cure rate using chemotherapy.
 - The researchers have prepared a library of three million compounds - or potential drug candidates (called ligands) and will use World Community Grid to simulate laboratory experiments to test which of these compounds block these proteins.









The Clean Energy Project

- Launched December 2008
- Sponsored by the Aspuru-Guzik group at Harvard University
- The main goal of the project is to calculate the electronic properties of tens of thousands of new materials and to determine which of these are the best candidates to make the next generation of affordable solar cells.
 - The fossil fuel based economy of the present must give way to the renewable energy based economy of the future, but getting there is the greatest challenge humanity faces. Chemistry can help meet this challenge by discovering new materials that efficiently harvest solar radiation, store energy for later use, and reconvert the stored energy when needed.
 - Researchers are employing molecular mechanics and electronic structure calculations to predict the optical and transport properties of molecules that could become the next generation of solar cell materials.









Nutritious Rice for the World

- Launched May 2008
- Sponsored by the University of Washington Data Center
- Project will create the largest and most comprehensive map of the structure of rice proteins and their related functions
 - Help agriculturalists and farmers pinpoint which plants should be selected for crossbreeding to cultivate better crops that produce more rice grains, ward off pests, resist disease or hold more nutrients.
 - Knowledge gained can be easily transferred to wheat and corn.
- Rice is the main food staple of more than half of the world's population.
 - Every year, 10 million people die of hunger and hunger-related diseases.









Help Conquer Cancer

- Launched November 2007
- Sponsored by the Ontario Cancer Institute (OCI), Princess Margaret Hospital and University Health Network
- The project will improve the results of protein X-Ray crystallography in order to increase understanding of cancer and its treatment.
 - X-Ray crystallography will enable researchers to determine the structure of many cancer-related proteins faster, leading to improved understanding of the function of these proteins, and enabling potential pharmaceutical interventions to treat this deadly disease.









Discovering Dengue Drugs - Together

- Launched August 2007
- Sponsored by sponsored by the University of Texas Medical Branch and the University of Chicago
- The project will complete extensive calculations to identify new drug–like molecules with potent antiviral activity against viruses that belong to the family called Flaviviridae,

which include dengue, hepatitis C, West Nile, and Yellow fever viruses.

 Calculations will accurately determine how tightly small drug–like molecules bind to the different flavivirus proteases.
Compounds predicted to bind tightly to viral proteases will be tested for anti–flavivirus activity.









FightAIDS@Home: Phase 1 and 2

"World Community Grid has enabled my lab Scripps to engage in research projects that we would not have attempted in the absence of this powerful public computing grid. It's allowed us to complete complex work in six months that would have taken five years."

- Professor Arthur Olson, Scripps Research Institute

- Sponsored by the Scripps Research Institute.
- Phase 1: Launched November 2005 to identify new inexpensive and effective anti-HIV drugs based on molecular structure
- First stage completed with over 2 quadrillion calculations processed.



- Virtually screened 2,000 drug compounds and discovered potential leads.

- Leads are being presented to chemists for the design of better drugs that can be used in clinical trials.

- **Phase 2:** Virtually screening 230,000 compounds against wild-type HIV protease
 - Scripps has already identified 40 chemicals that merit further laboratory testing and several of these have gone to the second phase of testing, moving closer to potential drugs.
- Four additional experiments in development





Human Proteome Folding Project: Phase 1 and 2

- Phase 1: Sponsored by the Institute for Systems Biology
- Launched November 2004 and completed July 2006
 - Produced a database that describes the structure of approximately 120,000 protein domains that could not be described previously using traditional approaches.
 - Database of protein structures is helping scientists take the next steps to understanding how diseases that involve these proteins work and, ultimately, how to cure them.
- Research would have taken 100 years, but was completed in 12 months with World Community Grid.
- Phase 2: Sponsored by New York University
- Launched October 2006
 - Focusing on a small number of proteins that are key markers for diagnosis and impact, with a special focus on proteins linked and cancer.
 - One particularly interesting research effort is examining the manner by which malaria is transmitted by nursing mothers to children.







AfricanClimate@Home

- Phase 1: Launched September 2007 completed July, 2008.
- Sponsored by the Climate Systems Analysis Group, University of Cape Town, South Africa
- The project will lead to the identification of combinations of key parameterizations that best simulate the varying climates of Africa.
 - More accurate models will give researchers a better understanding of the implications of various natural and manmade influences on the African climate.
 - Policy makers can then make important adaptation and mitigation decisions related to agriculture and water (e.g., planning irrigation infrastructures and promoting appropriate drought resistant crops on the best available information.









Genome Comparison Project

- Launched November 2006 and completed in July 2007
- Sponsored by Fiocruz (Brazil)
- Performing pair-wise comparisons among and between all genes for all sequenced organisms (from human beings to fruit flies to yeast)
- Building database of the results which will be available to the research community
 - Provides a huge headstart in understanding what these proteins do, how they play a role in disease processes, and ultimately in understanding how to devise a drug to combat a disease involved with the particular protein in question.









Help Defeat Cancer

- Launched July 2006 and completed June 2007
- Sponsored by The Cancer Institute of New Jersey, Rutgers University and UMDNJ – Robert Wood Johnson Medical School
- Long-term goal: Improve understanding of the underlying mechanisms of cancer to improve treatment and therapy planning for cancer patients.



- World Community Grid helped accelerate research to detect and track subtle changes in measurable parameters that could facilitate the discovery of prognosis clues, which are not apparent by human inspection or traditional analysis alone.
 - Researchers have created a web-based, robotic prototype to automatically image, analyze, archive and share tissue microarrays.
 - Initial focus: breast cancer, followed by head and neck cancers





How are research projects selected?

- Researchers interested in running on World Community Grid fill out a proposal available on our website
- Projects selected must meet the following requirements:
 - Must be from a not-for-profit organization
 - Research must have a humanitarian focus
 - Be suitable for running on a volunteer grid
 - Commit to placing the results computed into the public domain



echnology solving problems

World Community Grid Project Proposal

Please complete this form and return it to the email address below. Applications will only be accepted in the following formats: Microsoft® Word documents, <u>pdf</u>, <u>odf</u>, or <u>ascii</u> files. If you have any questions, please send your questions, along with your telephone number, to the email address below. Submit to e-mail address: rfp@worldcommunitygrid.org

Project name:

Project short description: _

Organization name: _

Principal investigator:

Principal Investigator's e-mail address:

Principal Investigator's mail address: Principal Investigator's telephones (office, fax, cell):

Date of submission:

Please write two project abstracts, one using layperson terminology and another for peer research scientists. Include a statement of the problem, the solution, how World Community Grid would accelerate progress, and how the project would help humanity and the world.

Abstract 1 (Scientific peer version):





The vision of CCC participation



- Leverage 5+ years of volunteer computing knowledge and process development
- A platform to run research when no other resources are available.









www.worldcommunitygrid.org

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