



world community grid

NEWSLETTER

Issue 3
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Our Vision: A healthier world.

Our Mission: Accelerating science by creating a supercomputer empowered by a global community of volunteers.

The Numbers:

- 19 years of WCG
- 2.51 million years of computation
- 810,516 volunteers
- 7,652,413 devices
- 32 projects benefited

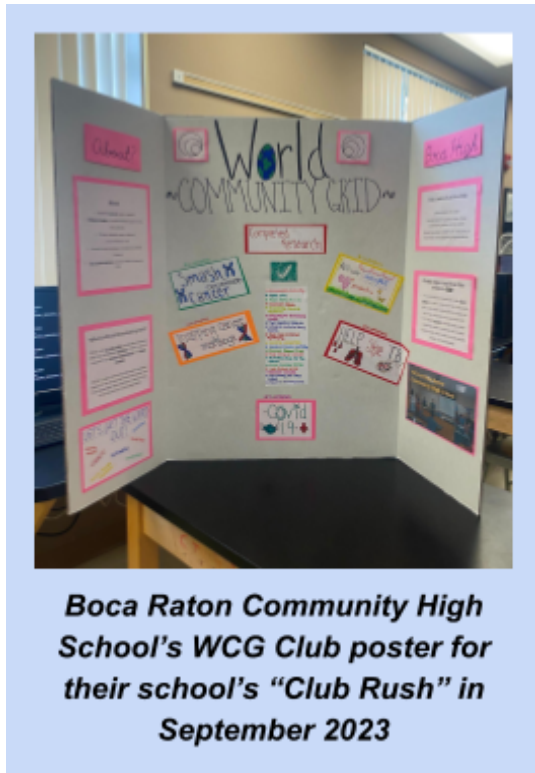
HIGH SCHOOL OUTREACH

The World Community Grid is a public, high performance computing platform enabling advanced open science and open data research that benefits humanity. While our scientific partners, funding partners, contributing partners and volunteers enable us to answer some of the world's most pressing questions by reducing required computational time, our partnerships with high schools and universities enable us to prepare the next generation for the future of scientific discovery. World Community Grid has the ability to enrich students' education and empower them to contribute to advanced research.

This year, we plan to expand our outreach program and to develop several new high school partnerships. This opportunity is open to all high schools, but in particular we are excited to extend partnerships to high schools in remote communities where access to educational institutions that can foster students' learning about high-performance computing and broad research fields may be limited. If you are a teacher or student who is interested, or if you know of someone who might be, please contact us directly.

Our existing high school partnerships include [Sisler High School Cyber Academy](#) in Winnipeg, Manitoba, Canada, and [Boca Raton Community High School](#) in Palm Beach County, Florida, United States. WCG has been seamlessly integrated into their classrooms and extracurricular activities to enrich student learning. For example, Sisler Cyber Academy first integrated WCG into their curriculum through an assignment enabling students to run WCG on several computers. In 2019, a

passionate student from Sisler Cyber Academy and his teacher, Mr. Esposito, visited the Krembil Research Institute in Toronto, Ontario, Canada, becoming the first WCG volunteers to meet Dr. Jurisica's team on-site. As students' interest in WCG grew, this led to the development of a WCG club which teaches students about how to set-up high-performance computing clusters, participates in WCG and supports scientific discoveries, sparks conversation about new developments from research initiatives, and hosts grid computing competitions. To learn more about WCG's involvement at Sisler Cyber Academy, read our [article](#) on outreach at this school.



At Boca Raton Community High School, students have also started a WCG club and interest in this club has grown so much that over 130 students signed up to learn more about WCG at their "Club Rush" this year. WCG has also been integrated into their science curriculum through presentations on research projects supported by the WCG projects. You can read more about outreach at this high school in our [article](#) on Boca Raton's WCG club.

Beyond these examples of WCG's high school partnerships, we are exploring new outreach options in the upcoming year. For example, we have started exploring the option of working with high schools' co-op programs and linking to their volunteering programs, as all high schools in Ontario

require volunteering experience. We also offer opportunities for students to develop scientific writing skills. This will include opportunities for students to define scientific terms for a general audience, and to create content about WCG research projects for our social media accounts under the mentorship of university students. We are excited about these opportunities to expand our reach and to enrich the learning of the next generation. And as we are planning the expansion phase of WCG, any new volunteer and partner extends the ability to support more projects.

CURRENT PROJECT UPDATES

African Rainfall Project

The movement of data from the storage at SURF, a cooperation of educational and research institutes in The Netherlands, to Amazon Web Services, is almost finished. All data files have been moved and the final step is to check if indeed the files have been copied correctly. This is done by comparing so-called hashes, which are a sort

of a digital fingerprint of 128 bits or 16 characters. Even if one bit has changed during the copying, the hashes on both sides will be different. So far, not a single bit has gone astray after checking about 300 TB.

The next step is to make the files more easily accessible, which should not take too long. In the first instance, this will be a list of files and their coordinates and period covered. ARP team plans that at a later phase the files could be selected more interactively. What remains for the short term is finishing the last simulations for which we are very grateful to our volunteers. The expectation is still that all simulations will be ready by the end of this year.

Help Stop TB

We are excited that the HSTB team has moved locations over the summer to Loughborough (pronounced luf-bu-rah) University. Loughborough has particular strengths in AI and machine learning techniques, alongside a strong emphasis on health, being located nearby one of Astra Zeneca's previous sites in the UK. The team is hoping that this environment, and the collaborative atmosphere, will help strengthen the work for the Help Stop TB programme, providing new ideas and avenues to work on. Whilst the move has created some disruption for the HSTB project to get back up and running quickly with new work units, these are being worked on, alongside preparing the existing work for publication. The team has been transferring the existing scripts to new machines, and undergoing testing to confirm everything is still compatible and working.

Mapping Cancer Markers

The MCM team's research into *lung cancer* biomarkers identified 26 genes with top scores across all signatures considered. We have been working on characterizing these genes, including [VAMP1](#), [FARP1](#), [GSDMB](#), and [ADH6](#).



We continue exploring two kinds of *sarcoma* signatures, one to distinguish uterine leiomyosarcoma (ULMS) and undifferentiated pleomorphic sarcoma (UPS) from other histological subtypes, and one to distinguish all 7 histological subtypes in our sarcoma dataset from one another. We ran over 224 million work units for each of these, testing over 7.7 trillion signatures to distinguish ULMS and UPS from one another, and over 2.7 trillion signatures to distinguish all 7 histological types from one another.

As noted in the [September research update](#), our *ovarian cancer* results were dishomogeneous and therefore we have decided to run additional ovarian cancer work units. On September 26th, the sarcoma project was paused and we restarted ovarian cancer.

While we perform, improve and expand our analyses of the three types of cancers run so far, we are looking at the future datasets that will be used for MCM. We are compiling a priority list that will be shared with volunteers before we proceed.

Open Pandemics

The OPN team has selected about 30 molecules for experimental testing in the lab. These work units ran over the past few months and docked molecules manufactured by Enamine, ChemBridge, and ChemDiv. The selection was based on visual inspection of docked poses and also on whether or not the docked molecules interact with helicase in a way that resembles the binding mode of known ligands. These interactions consist mostly of hydrogen bonds and the positioning of polar groups in the binding pocket. Current work units dock Enamine molecules against Zika's NS5 protein. Lastly, the team would like to introduce a new member. Manuel Llanos joined the Forli lab as a postdoctoral researcher and will work on World Community Grid projects on various fronts, including preparation of work units and on the analysis of results.

Smash Childhood Cancer

Dr. Hoshino's and Dr. Keller's teams at Chiba University and cc-TDI.org have partial analysis back from volunteer-generated simulations of drug-protein docking for the rhabdomyosarcoma protein MyoD1 and the Ewing sarcoma protein FLI1. On the wet lab side, the compound hits from the PAX-FOXO1 studies computed when WCG was still supported by IBM have led to a new NIH R03 grant as well as an approved letter of intent to apply for a CRUK-NCI \$25M application (see details [here](#) about Team Koodac).

FUNDRAISING CAMPAIGN

We would like to thank you for donating computing power to support research projects and diminishing computational bottlenecks for open science. We are immensely grateful for the passion of the volunteers who support WCG and its mission to accelerate science.



Over the 19 years, 910,467 volunteers donated more than 2.5 million CPU-GPU/years of computation, and we highly appreciate your dedication. Over the last year, we have started the fundraising campaign (<https://www.cs.toronto.edu/~juris/jlab/mcm.html?tab=donations>) to support back-end operation of the WCG. As an academic group, we face significant financial (and technical) challenges in providing the same level of support to the global research community as IBM was able to. It is not sustainable to use only the lab research funds to support the operation of the WCG. From September 2021 till August 2023,

64% of the cost to run WCG came from the lab research funding (covering system administration, application developer, communications).

We need your support more than ever before. We continue to search for long-term partners that could help supplement research funding we use for supporting the operation of WCG. If you have some contacts that may help, please, let us know. If you could spare additional resources to support us, there are multiple ways of donating to WCG: <https://www.cs.toronto.edu/~juris/jlab/mcm.html?tab=donations>, which are highlighted below.

- ☐ One time donation directly to the WCG at UHN Foundation:
https://support.uhnfoundation.ca/site/Donation2?2740.donation=form1&df_id=2740&mfc_pref=T&set.SingleDesignee=2001
- ☐ Monthly donation directly to the WCG at UHN Foundation:
<https://www.cs.toronto.edu/~juris/jlab/mmd.html>
- ☐ Should you wish to receive a US tax receipt, please call UHN Foundation at 416-603-5300 or toll free at 1-877-846-4483 (UHN-GIVE).



Thank you! Together, we will provide the necessary platform for important research benefiting humanity.