對外合作組織與機構動態報導

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EXASCALE AND THE CITY

城市與百萬兆級運算領域

By Joan Koka • October 16, 2017

Walk around any city neighborhood and chances are it looks nothing like it did 20 years ago. Thanks to growing urbanization, cities globally are rapidly expanding and

報告摘要(KEY INFORMATION)

1. 當我們在城市漫步時，很可能會發現周遭所見和 20 年前截然不同。由於不斷加速的都市化過程，全球的城市都在快速擴張，這也解釋全球不斷成長的人口、GDP，以及溫室氣體問題。阿岡計量中心的科學家期待可以運用超級電腦，幫助都市發展規劃人員評估程式系統與過程之模型的可運用性。
2. 我們的銀河系裡有數千億顆恆星，而據估計，宇宙中大約也有同等數量的星系，充滿大量的恆星，每顆恆星都有自己的衛星系統，而在星星與星系之間又有各種氣體和星塵；另外尚有暗物質以其十分不同又神秘的形態存在。阿岡科學家運用次世代數據分析與模擬技術，分析太空望遠鏡觀測所得的精密數據，嘗試建構整個宇宙的模擬系統。
3. 10 月 6 日，比利時核能研究中心在世界太空週舉辦了歡慶比利時太空首航與研究 25 週年紀念。這個重要時刻，讓研究人員得以回顧兩位太空人的太空航程以及相關研究的進展，瞻望未來登上火星的可能性，並大力著重在年輕世代的科學培養。
4. 先前侵襲美國的颶風並未造成油價的上揚，但影響了美國石油產品的出口與液化石油氣的現價。而有關中國與英法等國將全面引入電動車的規劃，就長期而言，其未來政策與趨勢是否對石油的需求產生影響，仍需密切關注。
5. 產業預測指出，為供儲備綠電所需，電池的需求將持續增加。而雖說鋰電池在效能上表現優異，但若考慮單位儲電成本，史丹佛所開發之鈉離子電池有望成為更具成本效益之方案。

accounting for more of our world's population, gross domestic product and greenhouse gases.

Adapting a city to keep up with evolving needs is one of the greatest daily challenges that city planners, designers and managers face. They must consider how proposed changes will affect systems and processes such as our power grid, green spaces and public health facilities. They also need to understand how these systems and processes will influence each other.

Charlie Catlett wants to make their job easier by using the power of exascale – supercomputers that will be at least 50 times faster than those in use today. Catlett, a senior computer scientist at the U.S. Department of Energy's (DOE) Argonne National Laboratory and a senior fellow at the Computation Institute, a joint institute of Argonne and the University of Chicago, leads the *Multiscale Coupled Urban Systems* project, which will create a computational framework for urban developers and planners to evaluate integrated models of city systems and processes.

With this framework, city planners can better examine complex systems, understand the relationships between them and predict how changes will affect them. It can ultimately help officials identify the best solutions to benefit urban communities.

"We're focused on coupling models for urban atmosphere, building energy, socioeconomic activity and transportation, and we will later expand to energy systems models," Catlett said. "The framework will define what data will be exchanged between these models and how that data will be structured."

Once the framework is complete, city planners such as those within the City of Chicago's Department of Planning and Development can work with researchers to answer questions, raise their own and optimize design proposals.

"It's a whole new frontier for us," said Eleanor Gorski, the deputy commissioner of planning, design and historic preservation for the City of Chicago's Department of Planning and Development.

"I think the most valuable aspect for us in city planning is being able to see how different conditions and parameters can affect different systems," said Gorski. "For example, if you have a building that is 10 stories and the developers want to add five stories, one of the things we'd want to know is what effect that will have on transportation. Is it going to cause congestion? What we don't have, and what I'm interested in, are those links between the data and the influence that one system has over another."

Two models that Catlett and his collaborators are working to couple are EnergyPlus, a DOE program to model the energy demands of buildings, and Nek5000, a turbulence model that will track heat and airflow going through a city.

By pairing these two, researchers can, for example, capture how variations in local climate can influence heat transfer, ventilation and energy demands. From there, policy experts could propose ways to improve structure design in future developments.

First, however, researchers must determine what kind of information to share between models. Temperature, for example, is something Nek5000 could send to EnergyPlus, since air temperature naturally affects the temperature along building surfaces, as well as heating and cooling costs. Yet even though such models are connected, today most run independently, not generally coupled with others, Catlett said.

The coupling framework will also aim to incorporate data from sensory devices, like those used in Argonne's urban [Array of Things project](). These sensors measure key components of the environment, such as ultraviolet and infrared light, cloud cover, temperature and humidity. These measurements can validate and improve existing models.

"The framework is key to solving these problems. It will essentially act as a data cache (*short-term storage*) through which a model can feed and receive information from another model or obtain data from sensory devices," Catlett said.

One of the challenges is that simulations of models run at different rates. For example, simulating one hour of time with an atmospheric model may take a day of computing, while simulating the same amount of time with a building energy model may take half a second. To overcome this problem, researchers are examining various techniques.

"We're exploring ways to match speeds by experimenting with the resolution of the simulations and by redistributing the resources on the machines, for example, having the more time-intensive simulation run on more computer cores than the less time-intensive one," Catlett said.

Researchers are also examining how to make the framework flexible enough to handle a wide variety of models. With a more broad-based design, developers can use the framework to answer many different kinds of questions.

"To couple models, you'd traditionally have a laboratory such as Argonne or Oak Ridge develop a custom package. The problem is that it ends up being so specific that others can't work with it, even if they're trying to address similar questions. In that case, they have to get another custom package developed to address their study," Catlett said.

"With our framework, we can eliminate this duplication of effort, but only if we design it in a general way such that other researchers can plug in their model with any of the others," he said.

This project is funded by and is one of the applications of the Exascale Computing Project (ECP), a collaborative effort of the DOE Office of Science and the National Nuclear Security Administration, that seeks to provide breakthrough modeling and simulation solutions through exascale computing.

Laboratories participating in the *Multiscale Coupled Urban Systems* project include Argonne National Laboratory, Lawrence Berkeley National Laboratory, National Renewable Energy Laboratory, Oak Ridge National Laboratory and Pacific Northwest National Laboratory.

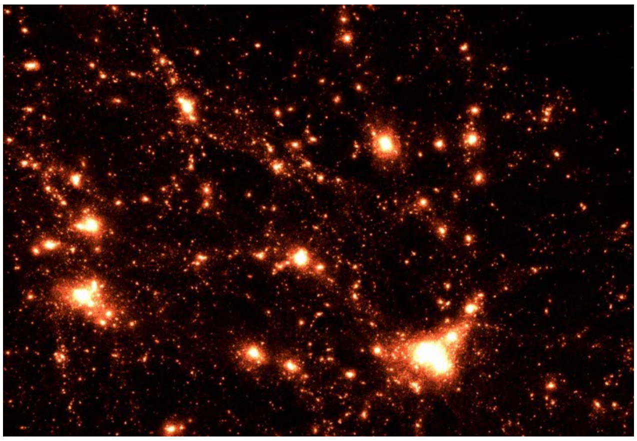
The Array of Things project is supported by the National Science Foundation, with additional support from Argonne National Laboratory and the Chicago Innovation Exchange.

CARTOGRAPHY OF THE COSMOS

宇宙製圖

By John Spizzirri • September 25, 2017

There are hundreds of billions of stars in our own Milky Way galaxy. Estimates indicate a similar number of galaxies in the observable universe, each with its own large assemblage of stars, many with their own planetary systems. Beyond and between these stars and galaxies are all manner of matter in various phases, such as gas and dust. Another form of matter, dark matter, exists in a very different and mysterious form, announcing its presence indirectly only through its gravitational effects.



This is the universe Salman Habib is trying to reconstruct, structure by structure, using precise observations from telescope surveys combined with next-generation data analysis and simulation techniques currently being primed for exascale computing.

"We're simulating all the processes in the structure and formation of the universe. It's like solving a very large physics puzzle," said Habib, a senior physicist and computational scientist with the High Energy Physics and Mathematics and Computer Science divisions of the U.S. Department of Energy's (DOE) Argonne National Laboratory.

Habib leads the "Computing the Sky at Extreme Scales" project or "ExaSky," one of the first projects funded by the recently established Exascale Computing Project (ECP), a collaborative effort between DOE's Office of Science and its National Nuclear Security Administration.

From determining the initial cause of primordial fluctuations to measuring the sum of all neutrino masses, this project's science objectives represent a laundry list of the biggest questions, mysteries and challenges currently confounding cosmologists.

There is the question of dark energy, the potential cause of the accelerated expansion of the universe, while yet another is the nature and distribution of dark matter in the universe.

These are immense questions that demand equally expansive computational power to answer. The ECP is readying science codes for exascale systems, the new workhorses of computational and big data science.

Initiated to drive the development of an "exascale ecosystem" of cutting-edge, high-performance architectures, codes and frameworks, the ECP will allow researchers to tackle data and computationally intensive challenges such as the ExaSky simulations of the known universe.

In addition to the magnitude of their computational demands, ECP projects are selected based on whether they meet specific strategic areas, ranging from energy and economic security to scientific discovery and healthcare.

"Salman's research certainly looks at important and fundamental scientific questions, but it has societal benefits, too," said Paul Messina, Argonne Distinguished Fellow. "Human beings tend to wonder where they came from, and that curiosity is very deep."

HACC'ing the night sky

For Habib, the ECP presents a two-fold challenge — how do you conduct cutting-edge science on cutting-edge machines?

The cross-divisional Argonne team has been working on the science through a multi-year effort at the Argonne Leadership Computing Facility (ALCF), a DOE Office of Science User Facility. The team is running cosmological simulations for large-scale sky surveys on the facility's 10-petaflop high-performance computer, Mira. The simulations are designed to work with observational data collected from specialized survey telescopes, like the forthcoming Dark Energy Spectroscopic Instrument (DESI) and the Large Synoptic Survey Telescope (LSST).

Survey telescopes look at much larger areas of the sky — up to half the sky, at any point — than does the Hubble Space Telescope, for instance, which focuses more on individual objects. One night concentrating on one patch, the next night another, survey instruments systematically examine the sky to develop a cartographic record of the cosmos, as Habib describes it.

Working in partnership with Los Alamos and Lawrence Berkeley National Laboratories, the Argonne team is readying itself to chart the rest of the course.

Their primary code, which Habib helped develop, is already among the fastest science production codes in use. Called HACC (Hardware/Hybrid Accelerated Cosmology Code), this particle-based cosmology framework supports a variety of programming models and algorithms.

Unique among codes used in other exascale computing projects, it can run on all current and prototype architectures, from the basic X86 chip used in most home PCs, to graphics processing units, to the newest Knights Landing chip found in Theta, the ALCF's latest supercomputing system.

As robust as the code is already, the HACC team continues to develop it further, adding significant new capabilities, such as hydrodynamics and associated subgrid models.

"When you run very large simulations of the universe, you can't possibly do everything, because it's just too detailed," Habib explained. "For example, if we're running a simulation where we literally have tens to hundreds of billions of galaxies, we cannot follow each galaxy in full detail. So we come up with approximate approaches, referred to as subgrid models."

Even with these improvements and its successes, the HACC code still will need to increase its performance and memory to be able to work in an exascale framework. In addition to HACC, the ExaSky project employs the adaptive mesh refinement code Nyx, developed at Lawrence Berkeley. HACC and Nyx complement each other with different areas of specialization. The synergy between the two is an important element of the ExaSky team's approach.

A cosmological simulation approach that melds multiple approaches allows the verification of difficult-to-resolve cosmological processes involving gravitational evolution, gas dynamics and astrophysical effects at very high dynamic ranges. New computational methods like machine learning will help scientists to quickly and systematically recognize features in both the observational and simulation data that represent unique events.

A trillion particles of light

The work produced under the ECP will serve several purposes, benefitting both the future of cosmological modeling and the development of successful exascale platforms.

On the modeling end, the computer can generate many universes with different parameters, allowing researchers to compare their models with observations to determine which models fit the data most accurately. Alternatively, the models can make predictions for observations yet to be made.

Models also can produce extremely realistic pictures of the sky, which is essential when planning large observational campaigns, such as those by DESI and LSST.

"Before you spend the money to build a telescope, it's important to also produce extremely good simulated data so that people can optimize observational campaigns to meet their data challenges," said Habib.

But the cost of realism is expensive. Simulations can range in the trillion-particle realm and produce several petabytes — quadrillions of bytes — of data in a single run. As exascale becomes prevalent, these simulations will produce 10 to 100 times as much data.

The work that the ExaSky team is doing, along with that of the other ECP research teams, will help address these challenges and those faced by computer manufacturers and software developers as they create coherent, functional exascale platforms to meet the needs of large-scale science. By working with their own codes on pre-exascale machines, the ECP research team can help guide vendors in chip design, I/O bandwidth and memory requirements and other features.

"All of these things can help the ECP community optimize their systems," noted Habib. "That's the fundamental reason why the ECP science teams were chosen. We will take the lessons we learn in dealing with this architecture back to the rest of the science community and say, 'We have found a solution.'"

25 YEARS AGO, THE FIRST BELGIAN WAS SENT INTO SPACE. IN THE FOOTSTEPS OF DIRK FRIMOUT AND FRANK DE WINNE, WILL YOU BE THE ONE TO FLY TO MARS?

第一位比利時人被送上太空是在 25 年前。 將來登上火星的會是你嗎？

This Friday, during the World Space Week, SCK•CEN celebrated the 25th anniversary of Belgian space flights and space research. The event was an opportunity to look back into the space flights of two Belgian astronauts, Dirk Frimout and Frank De Winne, but also into the scientific progress made and a promising future in which space travels to Mars are made possible. As part of this, Sarah Baatout, researcher at SCK•CEN, will go on a scientific mission to the Princess Elisabeth Antarctica in December.

The 25th anniversary attracted some 200 professionals, students and scientists to our research centre in Mol. SCK•CEN, the Belgian Nuclear Research Centre, plays a leading role in international research on the effects of exposition to ionizing radiation on the human body and its environment. Thanks to research on radioprotection, scientists are now getting a constantly better understanding of how the body of an astronaut works during space flights. Thanks to these technological advances, SCK•CEN contributes to the development of suitable applications so that, one day, travelling to Mars becomes possible.

“Belgian scientists and astronauts play an important role in research and development in the field of space exploration. Scientists and astronauts are working in close collaboration on current and future space discoveries. What we achieved in the last 25 years is incredible but we can achieve even more,” states Frank De Winne.

Scientific mission to Antarctica

SCK•CEN regularly sends experiments into space. Several major projects will be launched this autumn. In November, the first bioreactor of SCK•CEN will be sent to the International Space Station (ISS). Two weeks later, Sarah Baatout, head of unit Radiobiology at SCK•CEN, will take off for the Princess Elisabeth polar station where she will study the impact of extreme living conditions (containment, stress, remoteness, …) on the human immune system and will also perform research on the protective properties of spirulina as food supplement for astronauts. Through videoconferences, she will share her experience on a daily basis with students from various Belgian schools.

"Our scientific mission to Princess Elisabeth station is an important step forward for SCK•CEN and it will provide a lot of information for our space and medical research. Being able to share it with students on a daily basis really fills me with enthusiasm. I want to inspire youngsters for science and to encourage them to develop even further," explains Sarah Baatout, head of unit Radiobiology at SCK•CEN.

Youngsters: tomorrow's astronauts

In his speech, Dirk Frimout attached great importance to science and education. "Space expeditions have existed for 60 years and are of utmost importance for science, technology, economy and first and foremost for education. It is the duty of each astronaut to share his/her knowledge with the next generations. Space fuels the imagination of our youngsters and rouses their interest for science. In today's society, we are in need of youngsters with a scientific and technical background."

Students' imagination to infinity and beyond

Throughout the day, students from the kindergarten, primary and secondary sections of the European School in Mol have been showing tons of creativity to make papier-mâché helmets, drawings, rockets and space-related items. Several awards have even been granted to the astronauts in the making who also had the opportunity to ask questions to a real astronaut, Frank De Winne.

RECENT DEVELOPMENTS IN THE OIL AND LNG MARKETS

石油與液化石油氣之近期發展

By Yoshikazu Kobayashi

IEE JAPAN

The US was hit by two giant hurricanes in August and September, but oil prices were hardly affected, with WTI remaining in the higher $40/bbl range. Oil prices soared the last time two giant hurricanes hit in 2005, but this time, the market was apparently more conscious of the current supply glut and the decrease in demand resulting from the shutdown of hurricane-hit refineries.

The hurricanes, of course, did have some impact on the international energy market. As a result of a drop in refining capacity of almost 40% in the US Gulf Coast, US gasoline prices rose to more than a two-year high of $2.60/gallon, and due to a huge decline in exports from the Gulf Coast due to reduced refinery operation, Central and South American countries, which depend heavily on US products, are rushing to secure substitutes. The drop in exports from the Gulf Coast also contributed to the recent rise in international spot LNG prices mentioned later. If the Asian market grows more dependent on American LNG, Japan must prepare for the impact of hurricanes in this season as a significant risk for LNG procurement.

Prices remain low in the international oil market, but the demand-stimulus effect of the low prices is starting to appear on the demand side. The IEA has revised upwards its forecast for global oil demand growth for the third consecutive month since July 2017, and estimates growth of 1.6 million barrels year-on-year in the latest outlook. OPEC has also raised its estimate for global oil demand growth for 2017 by 150,000 bbl/day in the past two months to 1.42 million bbl/day year-on-year. Owing partly to these upward revisions, Brent has risen to the higher $50 range.

China is reportedly considering a ban on the sale of vehicles powered by internal-combustion engines in the country. While China is accelerating the switch to EVs as a government policy, the planned ban is unlikely to disrupt the country's oil demand soon, as it is not realistic to ban engine-powered vehicles in the near term with EVs accounting for just 1.5% of total vehicle sales as of 2016, and the domestic demand for gasoline accounting for just a quarter of the total domestic oil demand. However, this move confirms the Chinese government’s policy to accelerate the switch to EVs and reduce engine-powered vehicles, and should not be treated lightly. Together with Britain and France which announced this policy earlier, China's plans for introducing EVs and its actual progress continue to require close attention.

Spot LNG prices in Northeast Asia are rising to above $8/mmbtu at this time of writing. One of the reasons, in addition to the decrease in American LNG exports due to the hurricanes, is that spot LNG prices are now considered a bargain with the rise in oil and coal prices. As supplies start to come in from new projects, a further rise in prices is unlikely, but not entirely impossible if the new projects face production troubles as they did last year. The market is likely to remain volatile in the near term.

A STANFORD BATTERY BASED ON SODIUM MAY OFFER MORE COST-EFFECTIVE STORAGE THAN LITHIUM

史丹佛開發之鈉電池，其儲電成本效益可能較鋰電池為佳

By Tom Abate

As a warming world moves from fossil fuels toward renewable solar and wind energy, industrial forecasts predict an insatiable need for battery farms to store power and provide electricity when the sky is dark and the air is still. Against that backdrop, Stanford researchers have developed a sodium-based battery that can store the same amount of energy as a state-of-the-art lithium ion, at substantially lower cost.

Stanford researchers are developing a sodium ion battery based on a compound related to table salt. *(Image credit: Getty Images)*

Chemical engineer Zhenan Bao and her faculty collaborators, materials scientists Yi Cui and William Chueh, aren't the first researchers to design a sodium ion battery. But they believe the approach they describe in an Oct. 9 *Nature Energy* paper has the price and performance characteristics to create a sodium ion battery costing less than 80 percent of a lithium ion battery with the same storage capacity.

"Nothing may ever surpass lithium in performance," Bao said. "But lithium is so rare and costly that we need to develop high-performance but low-cost batteries based on abundant elements like sodium."

With materials constituting about one-quarter of a battery's price, the cost of lithium – about $15,000 a ton to mine and refine – looms large. That's why the Stanford team is basing its battery on widely available sodium-based electrode material that costs just $150 a ton.

This sodium-based electrode has a chemical makeup common to all salts: It has a positively charged ion – sodium – joined to a negatively charged ion. In table salt, chloride is the positive partner, but in the Stanford battery a sodium ion binds to a compound known as myo-inositol. Unlike the chloride in table salt, myo-inositol is not a household word. But it is a household product, found in baby formula and derived from rice bran or from a liquid byproduct of the process used to mill corn. Crucial to the idea of lowering the cost of battery materials, myo-inositol is an abundant organic compound familiar to industry.

Making it work

The sodium salt makes up the cathode, which is the pole of the battery that stores electrons.

The battery's internal chemistry shuttles those electrons toward the anode, which in this case is made up of phosphorous. The more efficiently the cathode shuttles those electrons toward and backward versus the anode, the better the battery works. For this prototype, postdoctoral scholar Min Ah Lee and the Stanford team improved how sodium and myo-inositol enable that electron flow, significantly boosting the performance of this sodium ion battery over previous attempts. The researchers focused mainly on the favorable cost-performance comparisons between their sodium ion battery and state of the art lithium. In the future they'll have to look at volumetric energy density – how big must a sodium ion battery be to store the same energy as a lithium ion system.

In addition, the team optimized their battery's charge-recharge cycle – how efficiently the battery stores electricity coming in from a rooftop solar array, for instance, and how effectively it delivers such stored power to, say, run the house lights at night. To better understand the atomic-level forces at play during this process, postdoctoral scholar Jihyun Hong and graduate student Kipil Lim worked with Chueh and Michael Toney, a scientist with the SLAC National Accelerator Laboratory. They studied precisely how the sodium ions attach and detach from the cathode, an insight that helped improve their overall battery design and performance.

The Stanford researchers believe their *Nature Energy* paper demonstrates that sodium-based batteries can be cost-effective alternatives to lithium-based batteries. Having already optimized the cathode and charging cycle, the researchers plan to focus next on tweaking the anode of their sodium ion battery.

"This is already a good design, but we are confident that it can be improved by further optimizing the phosphorus anode," said Cui.

Other members of the team included Stanford researchers Jeffrey Lopez, Yongming Sun and Dawei Feng. The work was funded by the U.S. Department of Energy's Advanced Battery Materials Research (BMR) Program. X-ray measurements were carried out at the Stanford Synchrotron Radiation Laboratory (SSRL), a national user facility operated by Stanford University on behalf of the U.S. Department of Energy, Office of Basic Energy Sciences.