CERN Project Sees Orders-of-Magnitude Speedup with AI Approach

By Rob Farber

August 14, 2018

An award-winning effort at CERN has demonstrated potential to significantly change how the physics based modeling and simulation communities view machine learning. The CERN team demonstrated that AI-based models have the potential to act as orders-of-magnitude-faster replacements for computationally expensive tasks in simulation, while maintaining a remarkable level of accuracy.

Dr. Federico Carminati (Project Coordinator, CERN) points out, “This work demonstrates the potential of ‘black box’ machine-learning models in physics-based simulations.”

A poster describing this work was awarded the prize for best poster in the category ‘programming models and systems software’ at ISC’18. This recognizes the importance of the work, which was carried out by Dr. Federico Carminati, Gul Rukh Khattak, and Dr. Sofia Vallecorsa at CERN, as well as Jean-Roch Vlimant at Caltech. The work is part of a CERN openlab project in collaboration with Intel Corporation, who partially funded the endeavor through the Intel Parallel Computing Center (IPCC) program.

Widespread potential impact for simulation

The world-wide impact for High-Energy Physics (HEP) scientists could be substantial, as outlined by the CERN poster, which points out that ”Currently, most of the LHC’s worldwide distributed CPU budget — in the range of half a million CPU-years equivalent — is dedicated to simulation.” Speeding up the most time-consuming simulation tasks (e.g., high-granularity calorimeters, which are components in a detector that measure the energy of particles[i]) will help scientists better utilize these allocations. The following are comparative results obtained by the CERN team in the time to create an electron shower, once the AI model has been fully trained:

Dr. Sofia Vallecorsa points out that the CPU based runtime is important as nearly all of the Geant user base runs on CPUs. Vallecorsa is a CERN physicist who was also highlighted in the CERN article *Coding has no gender (https://home.cern/about/updates/2018/02/coding-has-no-gender)*.

As scientists consider future CERN experiments, Vallecorsa observes, “Given future plans to upgrade CERN’s Large Hadron Collider, dramatically increasing particle collision rates, frameworks like this have the potential to play an important role in ensuring data rates remain manageable.”

This kind of approach could help to realize similar orders-of-magnitude-faster speedups for computationally expensive simulation tasks used in a range of fields.

Vallecorsa explains that the data distributions coming from the trained machine-learning model are remarkably close to the real and simulated data.

Time to create an electron shower

Method	Machine	Time/Shower (msec)
Full Simulation (geant4)	Intel Xeon Platinum 8180	17000
3d GAN (batch size 128)	Intel Xeon Platinum 8180	7

(https://6lli539m39y3hpkelqsm3c2fg-wpengine.netdna-ssl.com/wp-content/uploads/2018/08/hpc_creating_electro

Figure 1: Comparative runtime to create an electron shower of the machine-learning method (e.g. 3d GAN) vs. the full Monte-Carlo simulation (Image courtesy CERN)

A big change in thinking

The team demonstrated that “energy showers” detected by calorimeters can be interpreted as a 3D image[ii]. The process is illustrated in the following figure. The team adopted this approach from the machine-learning community as deep-learning convolutional neural networks are heavily utilized when working with images.

Use of GANS

The CERN team decided to train Generative Adversarial Networks (GANs) on the calorimeter images. GANs are particularly suited to act as a replacement for the expensive Monte Carlo methods used in HEP simulations as they generate realistic samples for complicated probability distributions, allow multi-modal output, can do interpolation, and are robust against missing data.

The basic idea is easy to understand: train a Generator (G) to create the calorimeter image with sufficient accuracy to trick a discriminator (D) which tries to identify artificial samples from the generator compared to real samples from the Monte Carlo simulation. G reproduces the data distribution starting from random noise. D estimates the probability that a sample came from the training data rather than G. The training procedure for G is to maximize the probability of D making a mistake. A high-level illustration of the GAN is provided below.

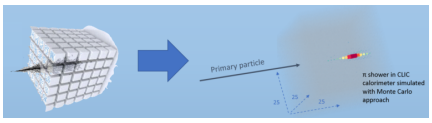

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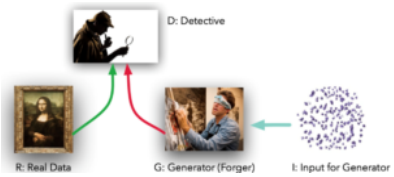
Figure 2: Schematic from the poster showing how a single particle creates an electron shower that can be viewed as an image (Courtesy CERN)

Even though the description is simple, 3D GANs are unfortunately not “out-of-the-box” networks, which meant the training of the model was non-trivial.

Results

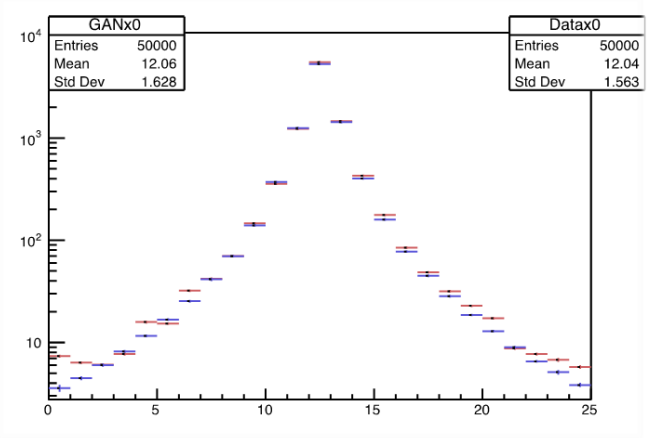
After detailed validation of the trained GAN, there was “remarkable” agreement between the images from the generator and the Monte-Carlo images. This type of approach could potentially be beneficial in other fields where Monte Carlo simulation is used.

More specifically, the CERN team compared high level quantities (e.g., energy shower shapes) and detailed calorimeter response (e.g., single cell response) between the trained generator and the standard Monte Carlo. The CERN team describes the agreement, which is within a few percent, as “remarkable” in their poster.

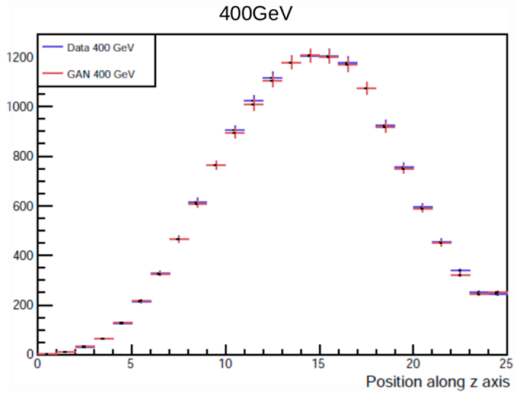


(https://6lli539m39y3hpkelqsm3c2fg-wpengine.netdna-ssl.com/wp-content/uploads/2018/08/hpc_training_a_gan.png)
Figure 3: High-level view of training a GAN (image from https://medium.com/@devnag/generative-adversearial-networks-in-50-lines-of-code-pytorch-e81b79659e3f (https://medium.com/@devnag/generative-adversearial-networks-in-50-lines-of-code-pytorch-e81b79659e3f))

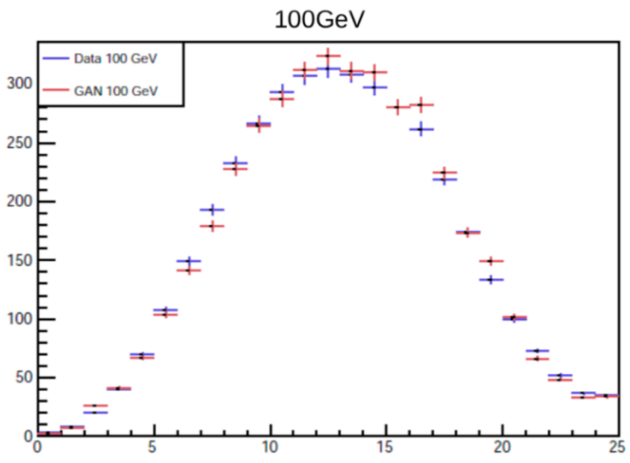
Visually this agreement can be seen by how closely the blue (real data) and red lines (GAN generated data) overlap in the following results reported in the poster.



(https://6lli539m39y3hpkelqsm3c2fg-wpengine.netdna-ssl.com/wp-content/uploads/2018/08/hpc_transverse_shower.png)
Figure 4: Transverse shower shape for 100-500 GeV pions. Red is the GAN data while blue represents the real data. (Image courtesy CERN)



(https://6lli539m39y3hpkelqsm3c2fg-wpengine.netdna-ssl.com/wp-content/uploads/2018/08/hpc_longitudinal_shower.png)
Figure 5: Longitudinal shower shape for 400 GeV electron (Image courtesy CERN)



(https://6lli539m39y3hpkelqsm3c2fg-wpengine.netdna-ssl.com/wp-content/uploads/2018/08/hpc_longitudinal_shower_more.fw_.png)
Figure 6: Longitudinal shower shape for 100 GeV electron (Image courtesy CERN)

Vallecorsa summarizes these results by stating, “The agreement between the images generated by our model and the Monte Carlo images has been beyond our expectations. This demonstrates that this is a promising avenue for further investigation.”

CERN openlab

The CERN team plans to test performance using FPGAs and other integrated accelerator technologies. FPGAs are known to deliver lower latency and higher inferencing performance than both CPUs and GPUs[iii]. The CERN group also intends to test several deep learning techniques in the hope of achieving a yet greater speedup with respect to Monte Carlo techniques, and ensuring this approach covers a range of detector types, which CERN believes is key to future projects.

This research is being carried out through a CERN openlab (https://openlab.cern/) project. CERN openlab is a public-private partnership through which CERN collaborates with leading ICT companies to drive innovation in cutting-edge ICT solutions for its research community. Intel has been a partner in CERN openlab since it was first established in 2001. Dr. Alberto Di Meglio (Head of CERN openlab) observes, “At CERN, we’re always interested in exploring upcoming technologies that can help researchers to make new ground-breaking discoveries about our universe. We support this through joint R&D projects with our collaborators from industry, and by making cutting-edge technologies available for evaluation by researchers at CERN.”

Summary

The HPC modeling and simulation community now has a promising path forward to exploit the benefits of machine learning. The key, as demonstrated by CERN, is that the machine-learning-generated distribution needs to be indistinguishable from other high-fidelity methods in physics-based simulations.

The motivation is straightforward: (1) orders of magnitude faster performance, (2) efficient CPU implementations, and (3) this approach could enable the use of other new technologies such as FPGAs that may significantly improve performance.

Additional References

- The award-winning CERN openlab poster (https://openlab.cern/sites/openlab.web.cern.ch/files/2018-06/Vallecorsa_poster.pdf).
- Goodfellow et al. 2014 (https://arxiv.org/abs/1406.2661)
- Conditional GAN, arXiv: 1411.1784 (https://arxiv.org/abs/1411.1784)
- Auxiliary Classifier GAN, arXiv:1610.0958 (https://arxiv.org/abs/1610.09585)
- The CERN team noted that all tests were run with Intel optimised Tensorflow (https://software.intel.com/en-us/articles/intel-optimization-for-tensorflow-installation-guide)4.1. + keras (https://keras.io/) 2.1.2

Rob Farber is a global technology consultant and author with an extensive background in HPC and in machine learning technology that he applies at national labs and commercial organizations on a variety of problems including challenges in high energy physics. Rob can be reached at info@techenablement.com (mailto:info@techenablement.com)

[i] http://cds.cern.ch/record/2254048# (http://cds.cern.ch/record/2254048)

[ii] ibid

[iii] https://medium.com/syncedreview/deep-learning-in-real-time-inference-acceleration-and-continuous-training-17dac9438b0b (https://medium.com/syncedreview/deep-learning-in-real-time-inference-acceleration-and-continuous-training-17dac9438b0b)

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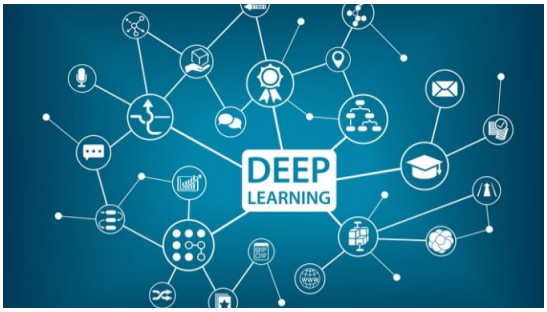
url=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F14%2Fnrel-eagle-supercomputer-to-advance-energy-tech-rd%2F)



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(https://www.hpcwire.com/2018/08/14/training-time-slashed-for-deep-learning/)

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learning%2F&title=Training%20Time%20Slashed%20for%20Deep%20Learning&source=https%3A%2F%2Fwww.hpcwire.com/) (http://www.faceboo
u=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F14%2Ftraining-time-slashed-for-deep-learning%2F&title=Training%20Time%20Slashed%20
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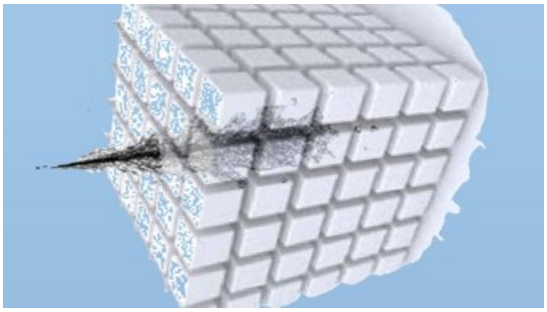

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An award-winning effort at CERN has demonstrated potential to significantly change how the physics based modeling and simulation communities view machine learning. The
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incorporates-ai-into-physics-based-simulations%2F) (http://www.linkedin.com/shareArticle?mini=true&url=https%3A%2F%2Fwww.hpcwire.com%2F2
simulations%2F&title=CERN%20Project%20Sees%20Orders-of-Magnitude%20Speedup%20with%20AI%20Approach&source=https%3A%2F%2Fwww.h
u=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F14%2Fcern-incorporates-ai-into-physics-based-simulations%2F&title=CERN%20Project%2
Magnitude%20Speedup%20with%20AI%20Approach/) (https://plus.google.com/share?url=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2

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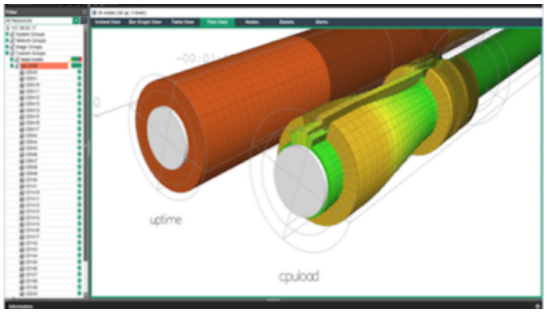

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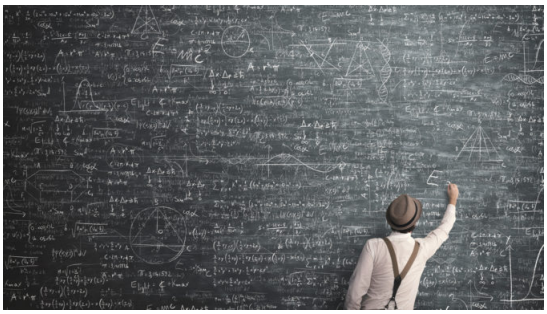

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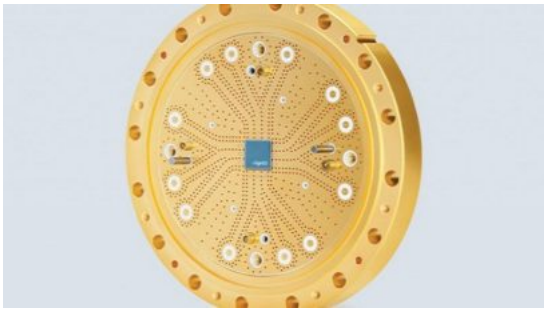

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Rigetti Computing plans to build a 128-qubit quantum computer based on an equivalent quantum processor that leverages emerging hybrid computing algorithms used to test p
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Intel Announces Cooper Lake, Advances AI Strategy

(https://www.hpcwire.com/2018/08/09/intel-advances-ai-strategy-at-data-centric-summit/)

Intel's chief datacenter exec Navin Shenoy kicked off the company's Data-Centric Innovation Summit Wednesday, the day-long program devoted to Intel's datacenter strategy, including another 14nm Xeon kicker, called Cooper Lake. Read more… (https://www.hpcwire.com/2018/08/09/intel-advances-ai-strategy-at-data-centric-summit/)

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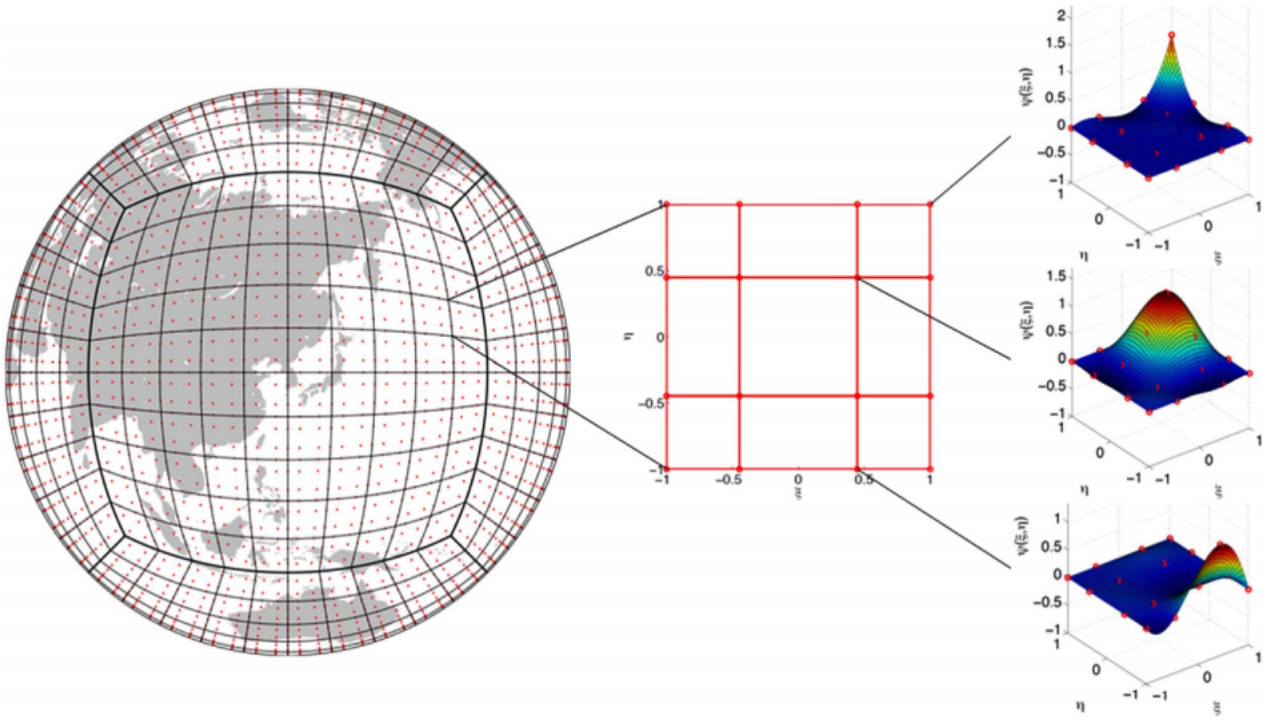
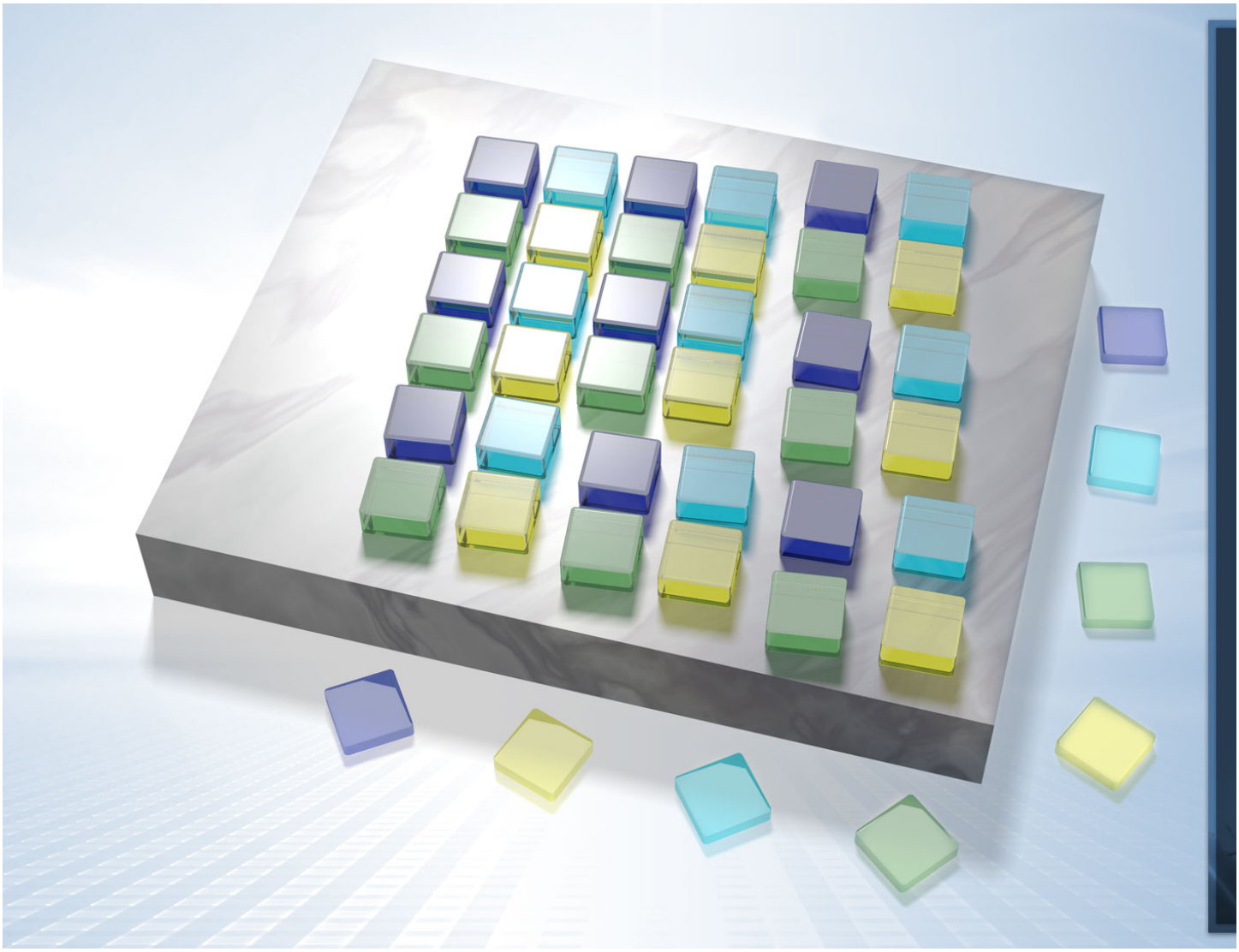


KIM, a New South Korean Global Weather Forecasting Model, Nears Deployment
(https://www.hpcwire.com/2018/08/09/kim-a-new-south-korean-global-weather-forecasting-model-nears-deployment/)

The United Kingdom Met Office's Unified Model (UM) has been in constant use around the world for over 25 years, serving – as its name suggests – as a unified hub for immed everything in-between. Read more… (https://www.hpcwire.com/2018/08/09/kim-a-new-south-korean-global-weather-forecasting-model-nears-deployment/)

By Oliver Peckham

(http://twitter.com/intent/tweet?status=KIM%2C%20a%20New%20South%20Korean%20Global%20Weather%20Forecasting%20Model%2C%20Nears%20Deployment+https%3A%2F%a-new-south-korean-global-weather-forecasting-model-nears-deployment%2F) (http://www.linkedin.com/shareArticle?mini=true&url=https%3A%2F%a-new-south-korean-global-weather-forecasting-model-nears-deployment%2F&title=KIM%2C%20a%20New%20South%20Korean%20Global%20Weather%20Forecasting%20Model%2C%20Nears%20Deployment& (http://www.facebook.com/sharer/sharer.php?u=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F09%2Fkim-a-new-south-korean-global-weathedeployment%2F&title=KIM%2C%20a%20New%20South%20Korean%20Global%20Weather%20Forecasting%20Model%2C%20Nears%20Deployment/url=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F09%2Fkim-a-new-south-korean-global-weather-forecasting-model-nears-deployment%2F)



SLATE Update: Making Math Libraries Exascale-ready
(https://www.hpcwire.com/2018/08/09/slate-update-making-math-libraries-exascale-ready/)

Practically-speaking, achieving exascale computing requires enabling HPC software to effectively use accelerators – mostly GPUs at present – and that remains something of
(https://www.hpcwire.com/2018/08/09/slate-update-making-math-libraries-exascale-ready/)

By John Russell

(http://twitter.com/intent/tweet?status=SLATE%20Update%3A%20Making%20Math%20Libraries%20Exascale-ready+https%3A%2F%2Fwww.hpcwi
making-math-libraries-exascale-ready%2F) (http://www.linkedin.com/shareArticle?mini=true&url=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F
exascale-ready%2F&title=SLATE%20Update%3A%20Making%20Math%20Libraries%20Exascale-ready&source=https%3A%2F%2Fwww.hpcwire.com/)
u=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F09%2Fslate-update-making-math-libraries-exascale-ready%2F&title=SLATE%20Update%3A
ready/) (https://plus.google.com/share?url=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F09%2Fslate-update-making-math-libraries-exa

Summertime in Washington: Some Unexpected Advanced Computing News
(https://www.hpcwire.com/2018/08/08/summertime-in-washington-some-unexpected-advanced-computing-news/)

Summertime in Washington DC is known for its heat and humidity. That is why most people get away to either the mountains or the seashore and things slow down. Read mor
washington-some-unexpected-advanced-computing-news/)

By Alex R. Larzelere

(http://twitter.com/intent/tweet?
status=Summertime%20in%20Washington%3A%20Some%20Unexpected%20Advanced%20Computing%20News+https%3A%2F%2Fwww.hpcwire.com
washington-some-unexpected-advanced-computing-news%2F) (http://www.linkedin.com/shareArticle?mini=true&url=https%3A%2F%2Fwww.hpcwir
washington-some-unexpected-advanced-computing-
news%2F&title=Summertime%20in%20Washington%3A%20Some%20Unexpected%20Advanced%20Computing%20News&source=https%3A%2F%2F
(http://www.facebook.com/sharer/sharer.php?u=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F08%2Fsummertime-in-washington-some-unex
news%2F&title=Summertime%20in%20Washington%3A%20Some%20Unexpected%20Advanced%20Computing%20News/) (https://plus.google.co
url=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F08%2Fsummertime-in-washington-some-unexpected-advanced-computing-news%2F)

Dell EMC Launches AI-Targeted Ready Solutions
(https://www.hpcwire.com/2018/08/08/dell-emc-launches-ai-targeted-ready-solutions/)

On Tuesday, Dell EMC announced Ready Solutions for AI, a technology stack intended to simplify AI and relieve organizations the drudgery of sourcing and piecing together th
(https://www.hpcwire.com/2018/08/08/dell-emc-launches-ai-targeted-ready-solutions/)

By Doug Black

(http://twitter.com/intent/tweet?status=Dell%20EMC%20Launches%20AI-Targeted%20Ready%20Solutions+https%3A%2F%2Fwww.hpcwire.com%2
targeted-ready-solutions%2F) (http://www.linkedin.com/shareArticle?mini=true&url=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F08%2
solutions%2F&title=Dell%20EMC%20Launches%20AI-Targeted%20Ready%20Solutions&source=https%3A%2F%2Fwww.hpcwire.com/) (http://www
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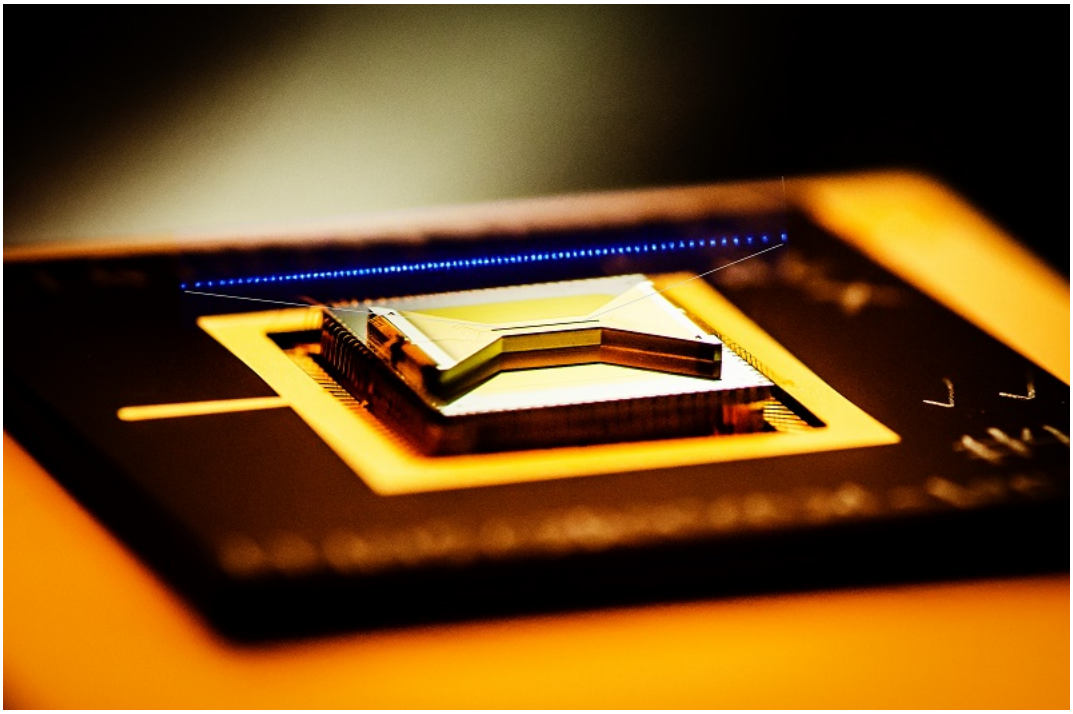
(https://plus.google.com/share?url=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F08%2Fdell-emc-launches-ai-targeted-ready-solutions%2F)

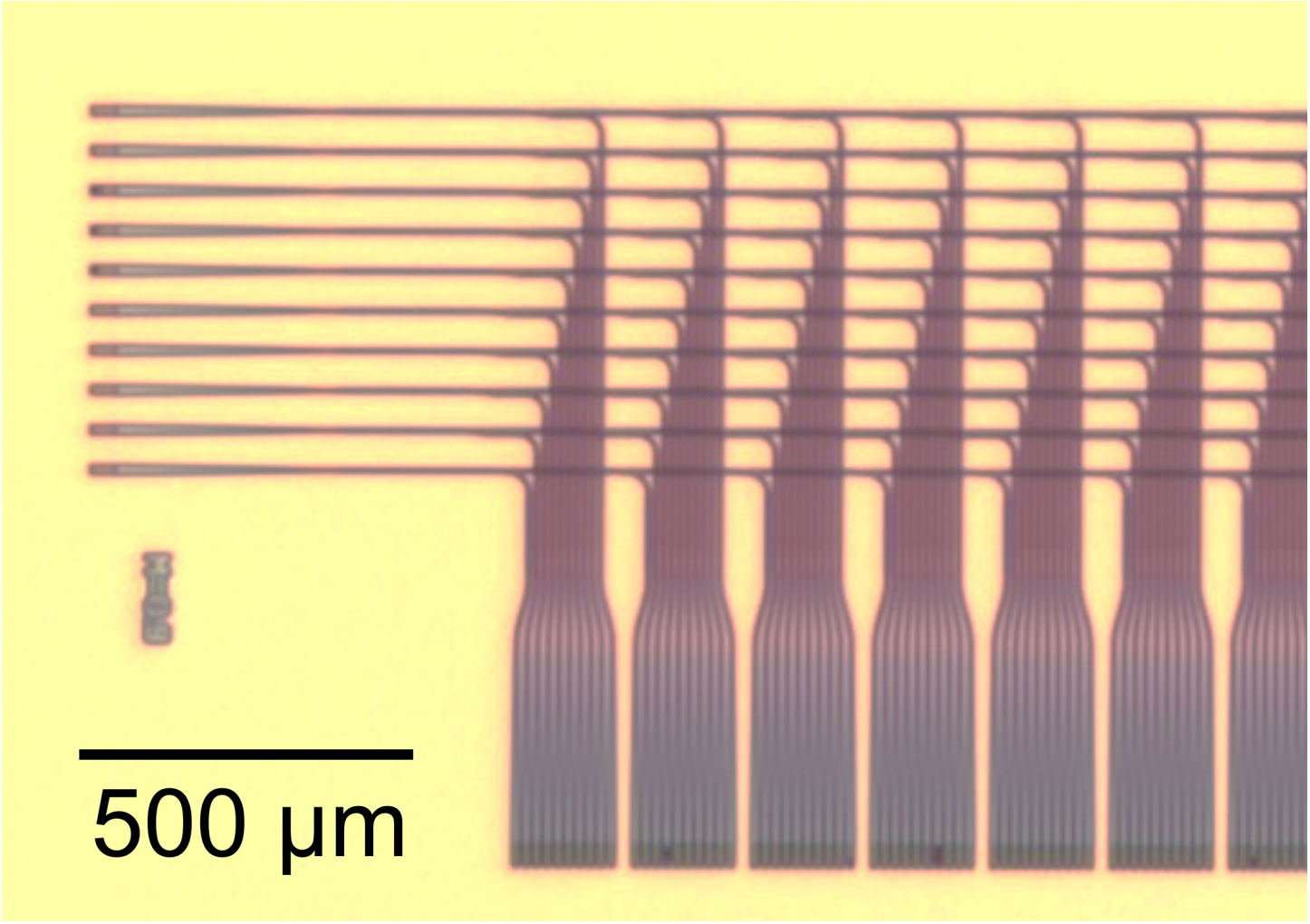


NSF Invests $15 Million in Quantum STAQ
(https://www.hpcwire.com/2018/08/07/nsf-invests-15-million-quantum-staq/)

Quantum computing development is in full ascent as global backers aim to transcend the limitations of classical computing by leveraging the magical-seeming properties of the problems in molecular modeling, cryptography and many other fields. Read more… (https://www.hpcwire.com/2018/08/07/nsf-invests-15-million-quantum-staq/)

By Tiffany Trader

(http://twitter.com/intent/tweet?status=NSF%20Invests%20%2415%20Million%20in%20Quantum%20STAQ+https%3A%2F%2Fwww.hpcwire.com%
quantum-staq%2F) (http://www.linkedin.com/shareArticle?mini=true&url=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F07%2Fnsf-invest
staq%2F&title=NSF%20Invests%20%2415%20Million%20in%20Quantum%20STAQ&source=https%3A%2F%2Fwww.hpcwire.com/) (http://www.fac
u=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F07%2Fnsf-invests-15-million-quantum-staq%2F&title=NSF%20Invests%20%2415%20Millio
(https://plus.google.com/share?url=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F07%2Fnsf-invests-15-million-quantum-staq%2F)



NIST Photonics Chip Breaks New Ground and Models Neural Net
(https://www.hpcwire.com/2018/08/07/nist-photonics-chip-breaks-new-ground-and-models-neural-net/)

Researchers at the National Institute of Standards and Technology (NIST) have made a silicon chip that distributes optical signals precisely across a miniature brain-like grid, s
more… (https://www.hpcwire.com/2018/08/07/nist-photonics-chip-breaks-new-ground-and-models-neural-net/)

By Staff

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status=NIST%20Photonics%20Chip%20Breaks%20New%20Ground%20and%20Models%20Neural%20Net+https%3A%2F%2Fwww.hpcwire.com%2F2
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models-neural-net%2F&title=NIST%20Photonics%20Chip%20Breaks%20New%20Ground%20and%20Models%20Neural%20Net&source=https%3A%2
(http://www.facebook.com/sharer/sharer.php?u=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F07%2Fnist-photonics-chip-breaks-new-ground
net%2F&title=NIST%20Photonics%20Chip%20Breaks%20New%20Ground%20and%20Models%20Neural%20Net/) (https://plus.google.com/share?
url=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F07%2Fnist-photonics-chip-breaks-new-ground-and-models-neural-net%2F)

Python Remains the Most Popular Programming Language
(https://www.hpcwire.com/2018/08/07/python-remains-the-most-popular-programming-language/)

Once again, Python is the most popular programming language according IEEE Spectrum's fifth annual interactive ranking of programming languages published last week. Re
remains-the-most-popular-programming-language/)

By John Russell

(http://twitter.com/intent/tweet?status=Python%20Remains%20the%20Most%20Popular%20Programming%20Language+https%3A%2F%2Fwww.h
remains-the-most-popular-programming-language%2F) (http://www.linkedin.com/shareArticle?mini=true&url=https%3A%2F%2Fwww.hpcwire.com%
popular-programming-language%2F&title=Python%20Remains%20the%20Most%20Popular%20Programming%20Language&source=https%3A%2F%2
(http://www.facebook.com/sharer/sharer.php?u=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F07%2Fpython-remains-the-most-popular-prog
language%2F&title=Python%20Remains%20the%20Most%20Popular%20Programming%20Language/) (https://plus.google.com/share?
url=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F07%2Fpython-remains-the-most-popular-programming-language%2F)

HPC Career Notes: August 2018 Edition

(https://www.hpcwire.com/2018/08/02/hpc-career-notes-august-2018-edition/)

In this monthly feature, we'll keep you up-to-date on the latest career developments for individuals in the high performance computing community. Read more… (https://www.h

By Oliver Peckham

(http://twitter.com/intent/tweet?status=HPC%20Career%20Notes%3A%20August%202018%20Edition+https%3A%2F%2Fwww.hpcwire.com%2F20 edition%2F) (http://www.linkedin.com/shareArticle?mini=true&url=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F02%2Fhpc-career-notes edition%2F&title=HPC%20Career%20Notes%3A%20August%202018%20Edition&source=https%3A%2F%2Fwww.hpcwire.com/) (http://www.faceb u=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F02%2Fhpc-career-notes-august-2018-edition%2F&title=HPC%20Career%20Notes%3A%20 (https://plus.google.com/share?url=https%3A%2F%2Fwww.hpcwire.com%2F2018%2F08%2F02%2Fhpc-career-notes-august-2018-edition%2F)

By the Numbers: Cray Would Like Exascale to Be the Icing on the Cake

(https://www.hpcwire.com/2018/08/01/cray-exascale-icing-on-the-cake/)

On its earnings call held for investors yesterday, Cray gave an accounting for its latest quarterly financials, offered future guidance and provided an update on potential exascal Read more… (https://www.hpcwire.com/2018/08/01/cray-exascale-icing-on-the-cake/)

By Tiffany Trader

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