SUCCESS STORY | SHELL

Using AI and HPC to Improve the Efficiency, Safety, and Sustainability of the Energy Sector

Image courtesy of Shell.

Shell's High-Performance Computing (HPC) Experts Collaborate with the NVIDIA AI Teams to Push Boundaries in the Energy Sector

Formed in 1907 as Royal Dutch Shell, with a foundation dating back to the 19th century, Shell is an international energy company with expertise in the exploration, production, refining, and marketing of oil and natural gas. Their advanced technologies and innovative approach won them the 2019 Award for Leadership in New Energy, given to organizations who stand out from their peers with bold investments and the goal of a clean energy economy.[1] Shell also has an ambitious target of being a net-zero emissions energy business by 2050.[2]

Shell has been using computational sciences to drive technology advancements since the 1960s. The computational sciences team's mission is to solve business problems—from developing better catalysts to better predicting the chemical reactions of materials to more accurately capturing flow through rocks, reactors, and pipelines. To do so, they are leveraging high-performance computing (HPC) to process and deliver real-time analytics, along with artificial intelligence to speed up analysis and interpretation. Collaborating with NVIDIA AI experts and using NVIDIA products has recently enabled Shell to generate better and faster insights in support of technological progress.

Shell uses NVIDIA AI to accelerate upstream activities in reservoir simulation and seismic processing. Image courtesy of Shell.

The computational sciences team at Shell supports their core business today and helps to build the energy companies of the future. Shell and NVIDIA worked together to deploy the NVIDIA DGX™ A100 to support improvements of specific HPC applications:

- Improve the human capital-intensive task of determining salt boundaries in hydrocarbon reservoir modeling by using Shell's proprietary AI algorithms
- Sharpen the accuracy of rock fluid property estimations in hydrocarbon reservoirs by enabling 4K iterative image reconstruction
- Test new designs for industrial plants to scale up the use of sustainable feedstocks, enabling the performance of computational fluid dynamics (CFD) simulations in days instead of weeks
- Drive advancements in sustainable new material development thanks to larger and faster molecular dynamics simulations

CUSTOMER PROFILE

Organization:	Industry:	Location:	Formed:	Website:
Shell	Energy	Global. Headquartered in The Hague, Netherlands, and London, U.K.	1907	www.shell.com/digitalisation

Shell's digital rock team visualizes micro-scale pore structure of rocks and runs flow simulations to predict reservoir behavior. Image courtesy of Shell.

Multi-Scale Modeling—from Pore to Reservoir Scale

One of the challenges in hydrocarbon extraction is to better understand the areas beneath the Earth's surface that are rich in oil and natural gas. Because these areas may also have huge deposits of salt, knowing the precise locations of these deposits is important for subsurface model building. As Vibhor Aggarwal, manager of HPC at Shell explained, "This is a very human-intensive and highly subjective task, where a seismic interpreter will manually pick salt boundaries. Improving the speed and accuracy of predictions enables us to maximize recovery from new and existing fields."

Vibhor's team collaborated with his Shell colleagues in the data science and subsurface community to accelerate 3D volume inference. They used a deep learning (DL) neural network to take a processed seismic volume and determine the locations of salt boundaries. Understanding the salt boundaries enabled a better interpretation of the flow of hydrocarbons, leading to the building of more accurate subsurface models. Using DL models helps Shell free up time for interpreters to focus on areas where their expertise adds more value.

The team already had NVIDIA DGX-2 systems based on NVIDIA V100 Tensor Core GPUs to speed up 3D volume inference. Each inference takes up to an hour to complete on a single seismic volume. To improve performance further, they turned to NVIDIA **DGX A100**[3] and leveraged AI containers from the NVIDIA **NGC™ catalog**[4] to help accelerate their training and inference workloads.

"Working with NVIDIA's team helped us improve our workflows. AI was doing inference on the volume, after which a human would look at it, tweak it, and re-run the inference job. If the inference takes too long, the loop becomes too long. DGX A100 has enabled us to shorten this loop considerably," says Vibhor. "Moving to DGX A100, we saw more than 2X improvement in inference performance with FP32 and an additional twenty to thirty percent improvement with automatic mixed precision (AMP)."

"With the DGX A100, single pass image reconstruction improved by 25 percent, while iterative reconstruction improved by 40 percent compared to the prior generation."

— Vibhor Aggarwal, Manager of HPC, Shell

Small Pores, Big Insights

Understanding the micro-scale pore structures of rocks provides insights into large-scale reservoir behavior, including where oil can be found and how best to extract it out of the ground. Shell's digital rock team takes micro computed tomography (micro-CT) images of rock samples to predict the properties of a reservoir, such as permeability and porosity. These characteristics provide input estimates related to the amount of hydrocarbon in the reservoir and what fraction of it can be produced.

With traditional experiments in the lab taking many months, there was a clear business case to replicate these experiments digitally. Shell's digital rock and computational sciences team built an end-to-end pipeline of applications leveraging GPUs—from taking micro-CT scans of core samples to doing 3D-image reconstruction and segmentation to running flow simulations.

The DGX A100 system is used to perform image reconstruction. "Before using GPUs, single pass image reconstruction was restricted by memory requirements and time constraints. With the DGX A100, single pass image reconstruction improved by 25 percent, while iterative reconstruction improved by 40 percent compared to prior generation," Vibhor said. Increasing the resolution of the pipeline, from reconstruction to segmentation to flow simulation, enabled Shell to predict the physical properties of rocks more accurately. The unique insights derived from such HPC usage drives more value out of each dollar invested in the discovery of new resources.

Going forward, Shell is looking to use AI to predict the physical properties from the pore structures of a given volume without running flow simulations.

Playing a Pivotal Role in Industrial Chemistry—from Fossil Fuels to Renewables

Beyond oil and gas exploration, Shell is investing in producing and supplying lower-carbon energy products and solutions. Oil is more than just for transportation fuel, it is being used to create just about everything from plastics, detergents, and even beauty products. Scientists break down hydrocarbons in oil and natural gas into simpler compounds and construct complex molecules.

Industrial reactors use hydrocarbons as feedstock and turn them into end products, like plastics and fuels, through chemical reactions. The computational sciences team at Shell supports the mission to design new reactors that use sustainable feedstocks, such as biomass, trees, plants, and recycled plastic.

The planning phase for a new manufacturing facility raises many questions about feedstock and product logistics, sizing of storage and process facilities, and the optimal operational model. Shell is using digital simulation to assess the best options. "Designing reactors requires experiments in pilot plants, where component size can stretch from inches to one foot in diameter. We use computational fluid dynamics (CFD) to predict what is happening in reactors. These CFD simulations help us understand and test designs before we build them," says Piet Moeleker, general manager of fluid flow and reactor engineering.

The DGX A100 helped the team conduct large, extensive CFD simulations. "When you scale simulations, you need to model hundreds of billions of particles. With DGX A100, we are working on reliably simulating reactors at commercial or near commercial scale before undertaking final investment decisions," Piet explained.

"The NVIDIA A100 Tensor Core GPUs are fast and reliable for tracking individual biomass particles in the reactors' fluid flow simulations," Piet said. "Calculations used to take two weeks. With the DGX A100, we can complete CFD simulations every five days."

The simulation methodology Piet's team leverages for traditional hydrocarbon processing can also be used to support the energy transition and applied across the development of new facilities, including wind farms or hydrogen plants.

"Calculations used to take two weeks. With the DGX A100, we can complete computational fluid dynamics simulations every five days."

— **Piet Moeleker,** General Manager of Fluid Flow and Reactor Engineering, Shell

Shell is committed to producing and supplying low carbon fuels (LCF) such as biodiesel and bioethanol to help lower carbon emissions from transportation. Image courtesy of Shell.

Better Living Through Sustainable Materials

Shell is also partnering with leading research institutes to push the technical boundaries of new material discovery. New materials can range from new drugs, food and personal care product ingredients, and ultra-low-cost and biodegradable plastic bottles, to components in electronic devices, such as elements of sensors and batteries. Shell's clean energy aspirations have led them to focus on new energy systems and sustainable chemistry, for example by looking into different electrocatalysts and the development of sustainable polymers.

Indranil Rudra, manager of computational chemistry and material science, works closely with Shell experimental laboratories to identify new leads for materials and predict the structure of properties and their performance. "Material discovery for business applications is currently driven by experimentation and a trial-and-error approach," Indranil explained. "The challenge is the robustness and transferability in off-the-shelf AI models for small material data sets. As such, we rely on computational chemistry and physics-based simulation to supplement experimental data."

For a new catalyst to be developed from lab to plant scale, it takes an average of 15 to 25 years—new material needs to be identified, followed by many cycles of synthesis and testing for different properties before production at scale.

With the DGX A100, the team reduces the timeline of laboratory activities by shortening the back-and-forth loop between computational output to experimentation to feedback. The computational chemistry and material science team uses the GPU version of VASP (Vienna Ab-initio Simulation Package), a software that performs molecular dynamics simulations. "Most calculations of VASP simulation take 42 to 72 hours to get structure optimization calculations completed. If that can be done within 24 hours, that loop can be made much faster," Indranil said.

"Using DGX A100, we saw an average speed-up of 2.5X on VASP's latest version when running structure optimization calculations vs CPU-only for a reasonable size system," Indranil explained. "Materials have billions of different molecular configurations, with useful materials being only a small portion of that. What was once too slow and too costly is now feasible and DGX A100 is helping us accelerate molecular discoveries."

"Using DGX A100, we saw an average speed-up of 2.5X on VASP's latest version when running structure optimization calculations vs. CPU-only for a reasonable size system."

— **Indranil Rudra,** Manager of Computational Chemistry and Material Science Team, Shell

Digital technologies are transforming the way Shell produces and supplies energy by improving the efficiency and safety of operations, and by advancing the use of renewable energy. "The timeline for developing new material spans several decades, but Shell is taking great strides in that direction," said Indranil.

Shell's wind farm turbines operate to produce clean power from an abundant, renewable resource. Image courtesy of Shell.

Towards a Sustainable Society

The computational science team is confident that their work can be a critical enabler of Shell's target to become a net-zero emissions energy business by 2050, in step with society's progress in achieving the goal of the UN Paris Agreement on climate change. Vibhor added, "Collaborating with others is an essential aspect of our strategy to bring in cutting-edge solutions and improve our use of HPC. Working with NVIDIA AI experts has helped us resolve performance issues and optimize the setup of the inference pipelines and software stack. This collaboration really helped us improve our utilization of our AI infrastructure."

Going forward, the team is also looking to use HPC systems for other use cases, such as weather modeling simulations, which is necessary to determine intermittency of power generation through wind and solar.

1 Energy Intelligence Forum. Royal Dutch Shell: Award for Leadership in New Energy 2019.
2 Shell. Our Climate Target.
3 DGX A100 is the universal system for all AI workloads - from analytics to training to inference - offering unprecedented compute density, performance, and flexibility, with 5 petaFLOPS of AI performance.
4 NVIDIA NGC catalog is a hub of GPU-optimized AI and HPC software..