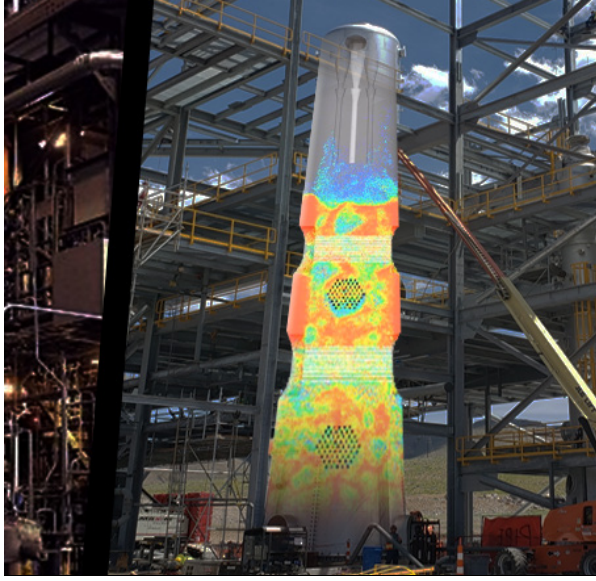
Solution Showcase

GPU-Parallelized Models Making a Green Impact

CPFD software simulations drive renewable technology innovation and speed time to market.



> "Leveraging high-performance computing, our clients can now better understand chemical and industrial processes, taking ideas that were once deemed impossible and making them a reality. This wouldn't be possible without technology partners like NVIDIA which enable us to speed up models and see into formerly opaque systems"
>
> **Peter Blaser**, Vice President of Operations, CPFD Software

Numerous technologies have been identified to help reduce the environmental impact and carbon footprint of energy-intensive industries. Unfortunately, the difficulty of demonstrating technological and commercial merit to potential partners, and the challenges of scaling from prototype to commercial viability, prevent most green energy solutions from achieving adoption at scale.

CPFD Software is changing that with its Barracuda Virtual Reactor® technology. Barracuda simulations enable organizations to validate and showcase the technological and commercial value of their sustainability solutions and reduce cost and time-to-market. This maximizes the likelihood of business success and widespread adoption of solutions that have a positive impact on our planet.

Barracuda Virtual Reactor: Researching, Developing, and Deploying Renewable Technologies

CPFD is a technology company in the field of computational fluid dynamics. Its flagship product, Barracuda Virtual Reactor, is a physics-based engineering software package capable of predicting fluid, particulate-solid, thermal, and chemically reacting behavior in fluidized bed reactors and other fluid-particle systems. With this visibility, organizations can reduce the risk associated with design, scale-up, commercialization, and troubleshooting of new and existing chemical and industrial processes.

CPFD makes simulation software in the field of computational fluid dynamics to help sustainability industry technology developers predict fluid, particulate-solid, thermal, and chemically reacting behaviors.

Industry

- Decarbonization
- Biofuel
- Circular economy

Challenge

- Demonstrating technological merit of innovations
- Proving commercial viability
- Scaling from lab to enterprise applications

Benefits

- Broaden scope of R&D through virtual testing
- Reduce physical testing cost
- Minimize development time and accelerate commercialization
- Showcase technical, practical, and commercial value

PREFERRED PARTNER

Fluidized bed processes are at the heart of myriad sustainability and decarbonization applications, such as the chemical recycling of plastics, production of biofuels, waste-to-fuel processes, carbon capture, and the hydrogen economy.

With the ability to virtually look inside industrial units like fluidized bed reactors, organizations developing renewable technologies can:

- Explore a wider range of possibilities during R&D
- Minimize the time and cost of physical testing
- Speed technology development
- Use simulations to communicate technical, practical, and commercial value to partners
- Scale up with confidence

To run Barracuda simulations containing trillions or more particles in a business-relevant time scale, CPFD has parallelized its models using NVIDIA® GPU technology and the NVIDIA CUDA® technology stack.

CPFD has received multiple awards in recognition of its contribution to the amplification of sustainable technologies, including "Best Software Technology" at the 2020 Hydrocarbon Processing Awards. CPFD is also a finalist in the Sustainability category for both the 2022 Hydrocarbon Processing Awards and the 2022 IChemE Global Awards.

GPU Acceleration

- 1,500X model speedups
- Yearlong simulations in less than one day
- Previously intractable problems now solvable

Awards

- Highly Commended at the 2020 IChemE Awards
- Best Software Technology at the 2020 Hydrocarbon Processing Awards
- Finalist in the **2022 IChemE Global Awards** in the categories of Sustainability and Process Automation and Digitalization

NVIDIA Products Used

- NVIDIA DGX™ systems

NVIDIA Software Used

- NVIDIA CUDA
- NVIDIA CUDA-X™

Barracuda Accelerates Commercialization for Chemical Recycling of Plastics

Plastic waste is one of the most serious environmental threats of our time. Of **400 million tonnes of plastic** produced each year, 91 percent is not recycled. Yet, eliminating plastic is not practical, nor even an environmentally friendly solution in many cases.

Using Barracuda Virtual Reactor, the University of Birmingham and its industrial partner, Recycling Technologies Ltd., have developed a **fluidized-bed-based plastics recycling system** that efficiently transforms plastic waste into valuable petrochemical fuels and virgin-quality plastic feedstocks. This eliminates the issues of degraded quality and impurities that limit the utility of traditional recycling of plastics.

Chemical recycling of plastics is a proven concept, but, until now, its practical application at commercial scale was not. This is where Barracuda Virtual Reactor comes in.

By comparing positron emission particle tracking data to Barracuda simulations, engineers were able to validate system flow patterns, velocity distribution, and circulation (turnover) rates. This enabled them to optimize system design to safely handle a wide variety of contaminated feedstocks.

Other CPFD partners using Barracuda Virtual Reactor to enable the chemical recycling of plastics include Anellotech and the Encina Development Group.

The Encina Development Group has integrated Barracuda simulations throughout its R&D to reduce risk and accelerate time to commercialization for its plastic fluid catalytic cracking process to convert mixed, hard-to-recycle plastics into circular chemicals. This world-first use for advanced recycling simulation, including the **largest simulation ever documented**, is reducing the need for fossil material while also reducing plastic waste. Encina is currently building a plant in Pennsylvania

> "Being nominated for the sustainability award is significant in recognizing our commitment to sustainability and the value Encina creates for our business, customers, and communities. [CPFD's] Virtual Reactor technology and expertise in fluidized beds are essential tools that enable us to meet Encina's technology objectives."
>
> **Carlo Badiola**, Senior Vice President of Engineering & Technology at Encina Development Group

that will process post-consumer materials into feedstocks that can be used to manufacture thousands of new products.

CPFD and Encina have been recognized as finalists in the **2022 IChemE Global Awards** in the categories of Sustainability and Process Automation and Digitalization for their work converting plastic waste into circular chemicals.

Anellotech, a sustainable technology company, is using Barracuda simulations to optimize the design of a commercial-scale fluidized bed reactor for its cutting-edge Plas-TCat™ process, a catalytic pyrolysis technology that chemically recycles mixed-waste plastics.

Anellotech has already built a fully automated pilot plant with a fluidized bed catalytic reactor, catalyst stripper, and regenerator that continually processes post-consumer plastic waste into aromatics and olefins—the raw materials required to manufacture plastics, detergent, adhesive, rubber, and food packaging.

> "Effective reactor design requires an understanding of the hydrodynamic and mixing parameters of the system as well as their effect upon the catalytic reactions. CPFD's Virtual Reactor software supports Anellotech's philosophy of model-based development, which reduces development time and scale-up risk."
>
> **David Sudolsky**, CEO of Anellotech

GPU-Accelerated Simulation Drives Waste-to-Jet-Fuel Process

ThermoChem Recovery International (TRI) has developed technology that converts municipal solid waste (MSW) and woody biomass into jet fuel. Starting in 2008, TRI began to digitize the development process with CPFD simulations.

TRI has been actively working with CPFD to model its steam reformer and validate the resulting Barracuda Virtual Reactor simulations in order to perfect the process of converting waste into sustainable fuel.

Using CPFD's Barracuda Virtual Reactor, TRI has tested and validated the full development path from cold flow studies to thermal profiling, chemical kinetics, and transport phenomena. Finally, TRI used Barracuda for commercial-scale reformer simulations.

Most recently, TRI's technology has been deployed by Fulcrum BioEnergy at a plant in Reno, Nevada, which converts 500 tonnes of MSW per day into jet fuel. The fuel is shipped directly to airlines, petroleum companies, and government purchasers.

Since the CPFD-TRI partnership began 14 years ago, TRI has benefitted from **1,500X model speedups** as CPFD moved its code from CPU hardware to full GPU parallelization, leveraging the latest NVIDIA hardware and software stack. With such exponential speedups, models that previously would have taken years can now be completed in a day or less.

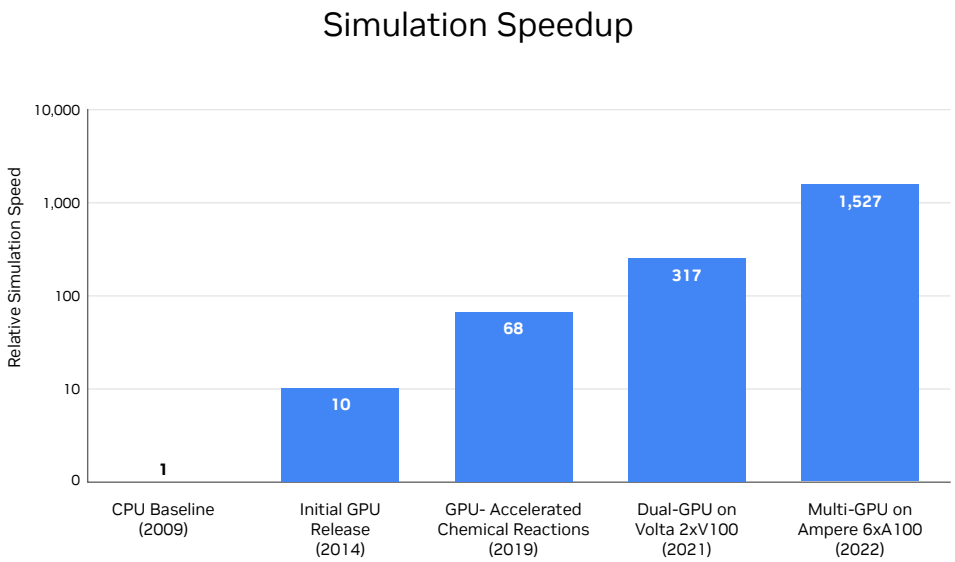


Figure 1: The chart to the left shows speedups gained with software and hardware improvements. TRI reported 2009-2019 speedup results at the Barracuda Virtual Reactor Users' Conference in 2019. The displayed 2021-2022 speedup results are based on in-house testing as confirmed by third-party benchmarks using cloud-served, multi-GPU resources.

CPFD and TRI were recognized with a Highly Commended designation at the **IChemE Awards in 2020** for their innovative work modeling deep fluid bed gasification to process waste and biomass into renewable fuels and chemicals.

GPU-Parallelized Models Powered by NVIDIA

By leveraging NVIDIA's CUDA framework and GPU systems, Barracuda Virtual Reactor software is able to simulate large-scale, industrial-sized units efficiently. Their multiphase particle-in-cell implementation has accelerated the flow solver, chemical reactions, and key particle operations with GPUs—processes that would be impractical to run on CPUs alone.

In 2021, CPFD added multi-GPU parallelization capabilities to its offering, enabling Barracuda Virtual Reactor to efficiently scale and run on NVIDIA DGX hardware systems. Users can now run simulations on up to eight NVIDIA A100 Tensor Core GPUs in a **DGX system** or four GPUs in a workstation that fits under a desk. Running a four-GPU workstation, simulations were completed 400X faster compared to a workstation powered by a single CPU.

For large-scale operations with massive datasets, Barracuda Virtual Reactor can run on NVIDIA HGX™ A100 GPUs, hardware specifically designed to handle simulation, data analytics, and AI workloads.

CPFD continues to take advantage of NVIDIA's latest technology releases. New benchmark results show Barracuda Virtual Reactor simulations experience a further 25 percent speedup running on NVIDIA H100 Tensor Core GPUs compared with the previous A100 generation.

To demonstrate the power of GPU speedups, CPFD revisited a 2012 simulation modeling 400,000 cells running on CPUs. The model would have taken three years to complete and was never finished. Today, a comparable model running on NVIDIA DGX systems can be completed in 13 hours.

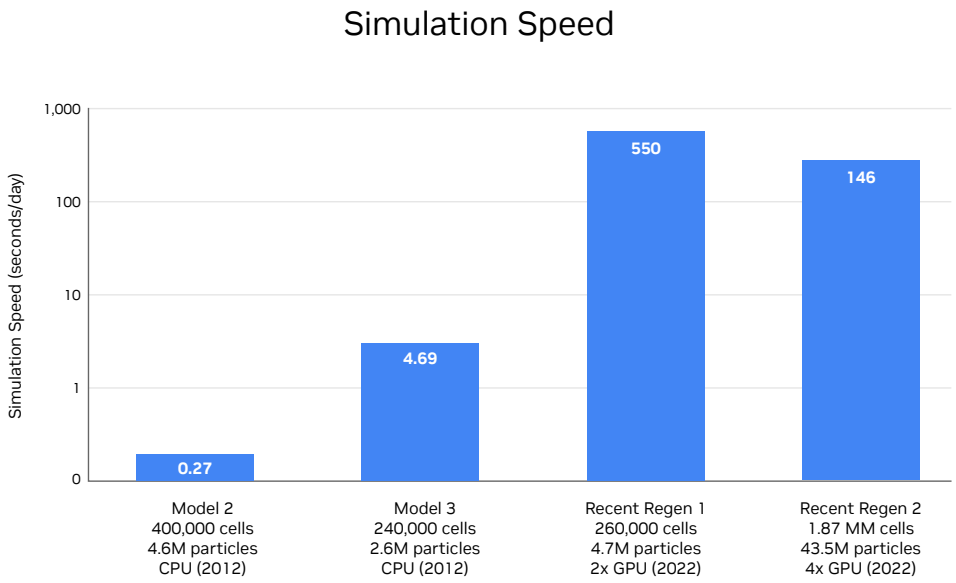


Figure 2. CPFD has used GPU speedups to complete large models in business-relevant timeframes. Models 2 and 3 were taken from an FCC regenerator simulation study, first created in 2012. Model 2 consisted of 400,000 cells and 4.6 million computational particles and would have taken approximately three years to complete using hardware and software technology available at that time. As a result, model 3 was created, which consisted of 240,000 cells and 2.6 million computational particles, with 2012 results available in about two months. Recent Regen cases 1 and 2 were similar models run in 2022 using two NVIDIA A100 GPUs, with results obtained in 13 hours and two days, respectively.

CFPD's Barracuda Virtual Reactor—Powered by NVIDIA

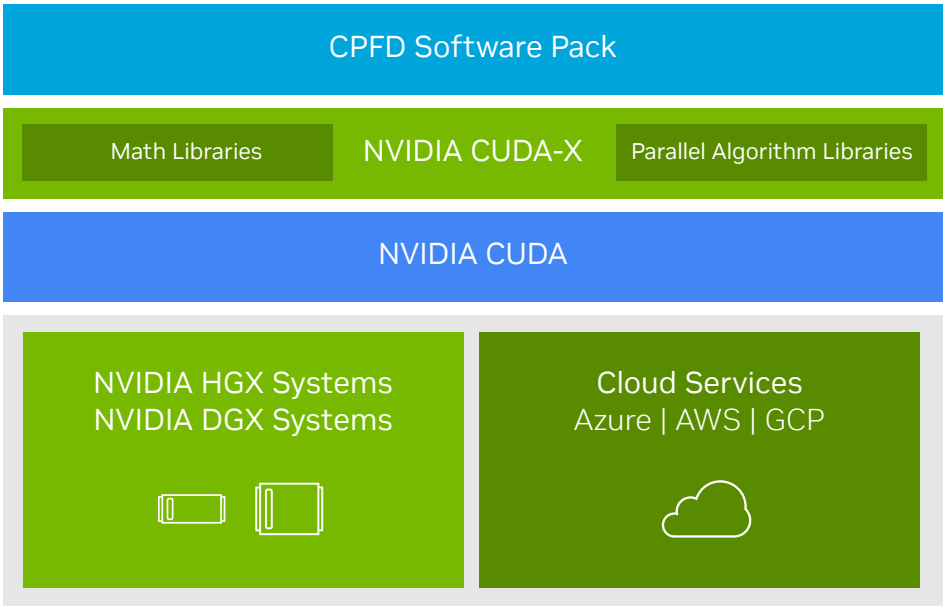


Figure 3. CPFD uses a parallelized code built on NVIDIA technology.

GPU speedups have transformed what is possible for the simulation of fluidized beds and innovation in sustainability and decarbonization technologies. Organizations working toward a greener planet can now run larger domain models with finer spatial resolution, more detailed physics, and more complex chemical reactions. Prior to the advent of readily available GPU and multi-GPU computing, such high-fidelity models simply could not be completed.

With CPFD's advanced simulations, clean energy innovators are increasing exploration of the research space, running fewer physical tests, reining-in development costs, and bringing impactful technologies to market faster.

Ready to Get Started?

To learn more about CPFD, visit:
cpfd-software.com/applications/clean-technologies

Learn how NVIDIA DGX systems are delivering AI-powered insights, visit: **www.nvidia.com/dgx**

NVIDIA