



FF4EuroHPC Success Story

# Optimal CO<sub>2</sub> Capture and Utilization Plant Design Through HPC

## Organizations

**Y Squared** is a Greek SME providing consulting services in the design of industrial chemical process systems, especially CO<sub>2</sub> capture and utilization systems.

**CERTH** is one of the top research centers in Greece and Europe, expert in HPC and CO<sub>2</sub> capture and utilization technologies.

**Yotta Advanced Computing** is a Croatian Hi-Tech SME, HPC expert, and provider.



End User



Technology Expert



HPC Provider



Centre for Research and Technology Hellas is part of the Greek NCC.



## The Challenge

The mitigation of greenhouse gas emissions is of utmost importance to eliminate their detrimental impacts on climate and the environment. One important step towards this aim is the availability of low-cost CO<sub>2</sub> capture and utilization (CCU) processes for intensely emitting industries, like the quicklime and cement sectors.

The design of the CCU systems is a computationally challenging task. Commercial, off-the-shelf tools have limitations such as handling each process for a nominal operating scenario sequentially and independently, and are often unable to use optimization algorithms or parallel computing effectively. This leads to costly designs, not motivating the wide industrial adoption of CCU.

Y Squared provides consultation services through tailored solution algorithms and computational procedures using systematic optimization and enabling simulations of multiple realistic operating scenarios. However, the need to search in larger design and operating spaces to find a globally optimum design which is cost effective and robust results in significantly longer computation time.





Industry Sector  
**Energy**

Technology used:  
**HPC**

## The Solution

The experiment has resulted in computational tools that combine algorithms for chemical process design and control with approximate computing and parallelization techniques. With the new tools, the discrete combination parameter space has increased by three orders of magnitude. The ability to solve the CCU problems simultaneously has reaped significant benefits compared to that of a sequential design approach. The computational time to obtain the optimal design has decreased by a factor of 50.

## The Impact

Y Squared is engaged in the design of CCU processes, primarily serving as a consultant for the cement and quicklime industries. The demand for CCU plants is expected to rise sharply due to the strict CO<sub>2</sub> regulations set internationally. The improved software provides Y Squared with a competitive advantage and market expansion opportunities in Greece and other European countries. The simultaneous design approach used in CCU resulted in a 6.5% lower cost per ton of calcium carbonate nanoparticles produced than the best, pre-project, sequential case. Due to the speed-up achieved by employing HPC, the company engineers managed to increase their efficiency and produce improved designs in a short amount of time. This allows Y Squared to take on more clients simultaneously and provide them with its customised and specialised services. The increased workload is expected to result in the creation of several job vacancies, as well as internship opportunities for young trainees to get exposure to chemical process design and modelling, advanced computing techniques, and HPC.

## Benefits

- HPC-aided CCU design achieves 6.5% cost reduction of calcium carbonate nanoparticles, making CCU more profitable.
- 1000x larger design spaces and 50x faster computing result in better designs which give Y Squared a competitive edge.
- 30% increase in revenue from design studies expected over the next 3 years.