We are *not on track* to meet the Paris Agreement's objectives. What should we do?

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The *Realistic* case for Gen AI

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The Realistic Case for Generative AI

1. Generative AI technology is mind blowing but not limitless, despite its rapid progress.
2. Even though building demonstrators is easy, scaling is hard. It requires quality data, integration with core IT, high levels of performance and change management.
3. High-value use cases are relatively few in number and require more than just a multi-agent based, multimodal large language model (LLM) to unlock value.
4. Gen AI can create tremendous value in the energy field, especially as it relates to energy transition.

Introduction

Even though Gen AI gained widespread public attention with the release of ChatGPT in 2022, its origins date back to the 1950s and extend far beyond language models in all their variations. It truly began to take off in the mid-2010s with the development of GANs, the first technology used to create deepfakes.

In 2023, there has been a bit of science fiction around the potential of the technology, be it in terms of impact on the global economy or the job market. After a year of frantic exploration, companies realized that scaling Gen AI is hard. It's time for for them to reset their approach with respect to Gen AI and remember the hard lessons learned from digital and AI transformation: steer by value; upskill people; set up the technology architecture; ensure data quality; and commit to the ethical and responsible development and use of Gen AI.

Moreover, the transformation brought by Gen AI should not be considered in isolation but alongside broader AI transformation efforts, with a strong emphasis on change management. Only by integrating these elements can the full value potential be realized, enabling deep process re-engineering and enhancing organizational efficiency.

In the energy industry, particularly in the context of the energy transition, Gen AI has a crucial role to play. It can act as a catalyst for discovery of e-fuels, contribute to the design of new batteries or wind turbines, advance synthetic biology, and provide augmented insights from multiple data sources to support better-informed decision-making.

What we are seeing

After a year of Gen AI potential exploration, most companies are taking a step back to take stock and determine which direction to move forward.

Companies are starting to realize that there may have been over-promises on the value creation potential of this technology and that scaling is much harder than planned. Scaling requires deep integration with core IT and existing tools, access to large knowledge and data corpuses of high quality (which quality is generally not high), numerous iterations to optimize the system prompt to minimize wrong or not relevant answers.

High-value uses cases need complex process re-engineering, coupling AI and Gen AI in agentic LLM workflows.

New catalysts discovery for e-fuel

About e-fuels

E-fuels are synthetic fuels made of carbon dioxide (or monoxide) and hydrogen, produced with decarbonized energy. They are alternative solutions, fungible in the energy system, to decarbonize sectors without alternatives, like long-range aviation. They are part of the toolbox to achieve short-, medium-, and long-term climate objectives.

As new electrical energy vectors, e-fuels enable indirect electrification, particularly as it relates to the hardest-to-decarbonize sectors, such as heavy mobility (aviation and maritime fuels) and the chemical industry (transformation reagents). Additionally, they facilitate the recycling of unavoidable CO_2 emissions, like those from the cement industry.

However, those fuels are very expensive to produce, costing up to 100 times more than conventional petroleum[1]. To decrease those costs, a number of levers can be activated, especially:

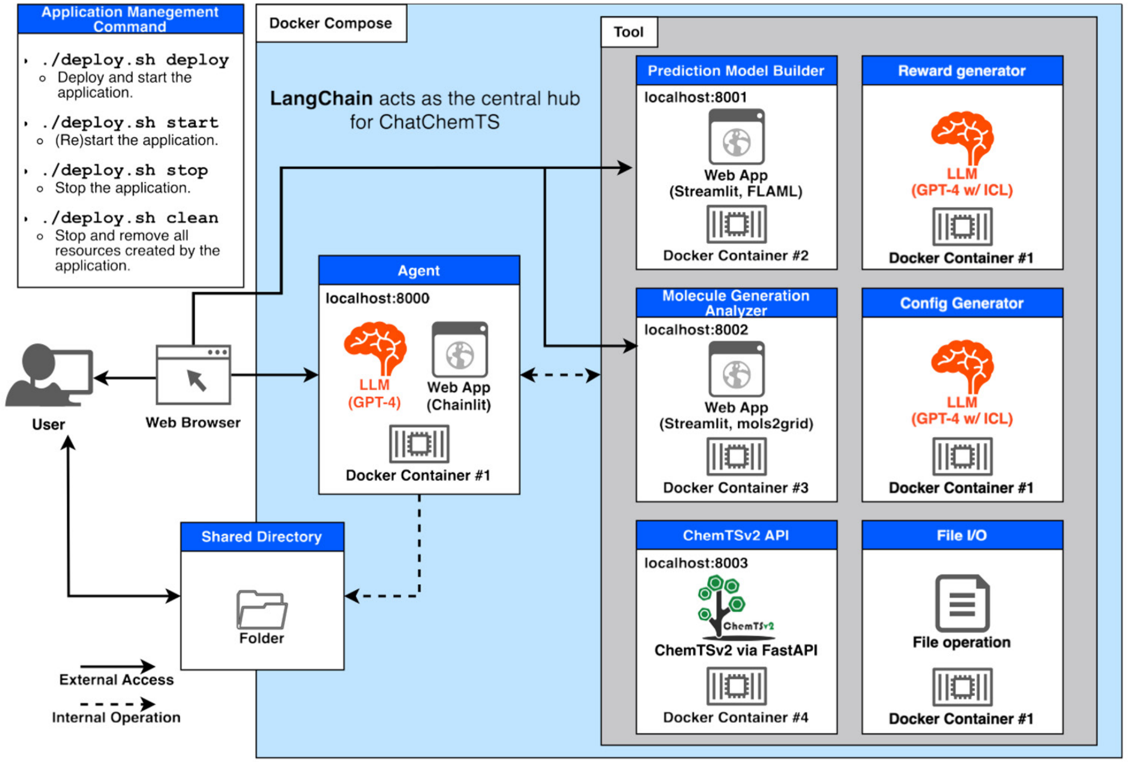
- the decarbonized electricity cost used to capture CO_2 and produce hydrogen
- the catalyst efficiency for the CO_2 to syngas reaction or for the Fischer-Tropsch reaction

One can leverage multi-agent LLM to orchestrate several highly specialized agents. one generates new formula, a second one predicts the desired properties for the application, in the case of catalysts, stability and activation energy) of the generated molecule. Finally, one can leverage the planning and reasoning ability of the Large Language Model to analyze the results and propose a new molecule.

Each reasoning step is performed until the LLM reaches an optimal point. It must be noted that experiments will still be required from time to time to constrain the prediction model and ground the LLM with real-world data. With such an approach, new catalysts may be suggested to the chemists in a few minutes, a limiting step in real-world experiments.

How Gen AI can be leveraged to accelerate e-fuels development?

Designing better catalysts is critical to lowering the global energy bill required to produce e-fuel and thus its production costs.



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1 https://www.pik-potsdam.de/members/Ueckerdt/E-Fuels_Stand-und-Projektionen_PIK-Potsdam.pdf

New batteries

About batteries

Batteries are an essential part of our energy transition journey. Obviously in EVs, they play a key role of decarbonizing lightweight vehicles. Moreover, battery energy storage systems (BESS) and large gigabatteries play a crucial role in ensuring electric grid stability as renewable energy sources and electric vehicle adoption rates increase. Indeed, due to the inherent intermittency of renewable electricity production and the growing use of charging stations, there may be significant stress on the electric grid. In such cases, large gigabatteries play a crucial role as buffers, stabilizing the grid until other measures can be activated to meet the demand.

For those batteries to be as efficient as possible, one must increase their energy density as well their power density. The first one is to increase the quantity of energy in the battery, while the second one is to increase the speed of charge/discharge.

How can Gen AI help in designing better batteries?[2]

As for e-fuels, Gen AI can be used to discover electrolytes with better properties to increase energy density. It can also be used to discover new binders that play a key role in dispersing the active material in the slurry and its adhesion to the current collectors to improve ionic and electrical conductivity.

To improve power density, one should play on the 3D porous network design optimization of the battery. In this step, we will rely on generative design approaches, where the engineers will specify the objectives and requirements of the final products, including manufacturing constraints.

2 https://interestingengineering.com/energy/lg-energy-solution-ai-battery-designing

Bio-engineered fuels through synthetic biology

About synthetic biology

Synthetic biology is an interdisciplinary field between biology, engineering, and computer science to design and build new biological systems or to re-design existing ones for new purposes. It involves the modification of organisms' genetic material to create novel functions that do not exist in nature. By applying engineering principles to biology, synthetic biology aims to make biological processes more predictable, scalable, and efficient. The field holds potential for innovations in healthcare, agriculture, environmental sustainability, and industrial manufacturing. It also raises ethical and safety considerations due to the power of reprogramming living organisms.

How Gen AI can be leveraged to accelerate new bio-engineered fuels ?

Traditional biofuels, such as ethanol from corn or biodiesel from vegetable oils, have limitations in efficiency, scalability, and environmental impact. Synthetic biology addresses these challenges by designing organisms that can convert a wider range of feedstocks, including non-food biomass, waste materials, and even carbon dioxide, into fuels.

One of the key advancements is the engineering of microbes to produce advanced biofuels like butanol, isobutanol, and fatty acid-derived fuels, which are more energy-dense and compatible with existing fuel infrastructures.

Synthetic biology enables precise control over metabolic pathways within these organisms, optimizing the conversion of sugars, cellulose, or other feedstocks into desired fuel molecules.

For example, engineered strains of E. coli or yeast can be designed to break down lignocellulosic biomass (plant material) into simpler sugars and then convert these sugars into biofuels. Additionally, synthetic biology can be used to create organisms that fix carbon dioxide and convert it directly into fuels or even convert directly feedstocks into hydrogen, offering lower carbon footprint alternatives.

Moreover, synthetic biology facilitates the rapid development and testing of new fuel-producing pathways through techniques like DNA synthesis, CRISPR-based genome editing, and metabolic modeling. This accelerates the discovery of efficient fuel production methods, reducing costs and increasing scalability.

Overall, synthetic biology's ability to engineer organisms for specific biofuel production processes holds the potential to revolutionize the energy industry by providing sustainable, renewable, and environmentally friendly alternatives to fossil fuels, contributing to energy security and the reduction of greenhouse gas emissions.

Our Convictions

- Generative AI technology, when coupled with AI, has the power to accelerate technology discovery for energy transition.
- As examples, those technologies can be used to
  - Discover new catalysts to convert CO_2 into fuels
  - Accelerate battery design to the 1-day scale
  - Design new living organisms that generate biofuels or biohydrogen with lower carbon footprints and much more robust processes
- However, one should not forget that those technologies are still generating substantial amount of wrong or irrelevant answers.
- Humans must verify through real world experiments that the designed molecules or systems do have the properties predicted by the agentic LLM workflow. If not, additional training phases, with reinforcement learning by example, will be required to improve the performance of the system.

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