Shrinking, cracking and flowing of porous media undergoing thermal conversion.
Design and implementation of the novel OpenFOAM library

Who does not know the enchanting warmth and glow of the campfire? All of us do. Most of us know the disappointment when the wood is gone, and the fire extinguished. But where did it go? How? And when did it happen?

This project aims to understand better how porous materials displace during thermal and chemical conversion. We are looking at pyrolysis, gasification and fire. These examples of conversion of porous media involve heat and mass transfer. Moreover, they are very important processes in renewable energy production, petrochemical synthesis, clean waste utilization and environmental catastrophes like wildfires. Other important examples of structurally evolving porous media include phenomena superficially different such as cave formation or nutrient transport in living tissues.
We build mathematical models and a computational tool which can evaluate those models. Although mathematical models are simplified, compact expressions that summarise features observed in experiments, in this case, they are far too complex to comprehend without suitable computational tools. The tool we develop is open-source, so everybody can use it without limitations. It is also part of the much bigger open-source library OpenFOAM, a popular tool for simulating fluid flows.
The first type of motion we investigate is the evolution of a single particle of biomass. Experiments show that a wooden stick will shrink, twist, and sometimes swell and break when set on fire. Qualitatively these phenomena can be observed in the example of a fire match. But only some know that a sufficiently large log of wood explodes when heated up sufficiently quickly. The mathematical relation between material composition, temperature, internal tensions and displacement should explain what stands behind the word sufficient and which features are crucial for the stability of the structure. The starting point for our analysis is careful and precise measurements of structure evolution in the process, including data as detailed as scanning electron microscopy of pores at the sample's surface and microtomography of the pores inside the samples.
The second type of motion we study is the dynamics of the bulk of particles, which obey the detailed single-particle dynamics. A special case of such a system is a campfire. The fresh wooden logs are typically put on top of it, and while they burn, they travel downwards, changing their shape, compressing the previously added logs and finally, they turn to ashes, which occupy about 1% of the volume of what was initially a log. The rest of the matter is carried to the atmosphere as $CO2$, CO, $H2O$ and other products of chemical reactions. This familiar process includes exciting and challenging physical phenomena like structure failure, granular motion, fluidization, and creeping motion. It is also vital to notice that during the porous medium's motion, neither mass of solid particles nor their volume are conserved, which makes it very interesting from the point of view of fluid mechanics models.
As a result, we will obtain an open-source platform for expressing realistic models and the realistic models of the motion of porous media upon their chemical and thermal conversion. The models will provide a novel understanding of the material's behaviour under thermal and chemical stresses. This is of importance for fire safety, environmental studies and industrial production. A good model should, e.g., inform actions that will lower $CO2$ emissions during peat fires. The platform itself will greatly help other scientists to study, test and parametrize the porous media motion models in other contexts.