Advancing numerical modelling for ultimate metamaterial design

“I have always worked at the boundary between computer science and engineering,” says Dr. Alejandro Aragón, assistant professor in the department of Precision and Microsystems Engineering at the Delft University of Technology. “Personally, I find it more rewarding to create a new numerical methodology that others can use to solve their problems, instead of just using an existing approach.” To this end, Aragón has recently developed highly advanced computational methods, which not only have the potential to improve the way discontinuities are analysed, but will also enhance the design of structures and new artificially engineered (meta) materials.

The Finite Element Method
Known about since the mid-twentieth century, the Finite Element Method (FEM) is a numerical procedure used to analyse problems in physics and engineering. FEM works by subdividing a large problem into smaller, simpler parts called finite elements. This discretisation process results in a so-called finite element mesh that is subsequently used for the analysis. Although the behaviour within each element is simple, once reassembled, they can reproduce very complex behaviour.

Enriched Finite Element Methods
In order to preserve accuracy, FEM relies on a "matching mesh", where the sides of the elements align with the problem geometry. However, Aragón has worked for years on creating ‘Enriched Finite Element Methods’ (EFEM) as a way to analyse problems with meshes that are independent of the problem’s geometric features. “This mesh-independent analysis is possible because you incorporate extra information about the solution within the analysis thereby 'enriching' the finite element formulation and thus regaining the accuracy missing by using a non-matching mesh,” explains Aragón.

Initially, his research efforts focused on solving problems with weak discontinuities, where “the gradient of the field is discontinuous, such as the temperature or the displacement field in materials composed by different phases,” says Aragón.

Discontinuity-Enriched Finite Element Method
Since moving to Delft, Aragón has created the ‘Discontinuity-Enriched Finite Element Method’ (DE-FEM). This computational technique can be used to model problems with both weak and strong discontinuities - cracks - and this technology can be extremely useful for the mesh-independent analysis of problems in fracture mechanics. “What it means is that I can have an object with any geometry, with an arbitrary number of material interfaces, and I can put cracks on top of that, and then I can solve that problem by immersing it in an FE mesh that is completely independent of all those discontinuities,” says Aragón. “I’m super excited about this as it’s a really new way to model these sorts of problems.” Moreover, the objective is to integrate this
advanced FE technology in the near future within optimisation for performing design. “And there’s a lot of knowledge in our Structural Optimization and Mechanics group in that direction,” adds Aragón.

**Metamaterials**
Importantly, Aragón has also been able to apply these advanced numerical technologies to help design new metamaterials – materials, which are artificially engineered to control and manipulate certain physical properties. Metamaterials get their ‘unnatural’ properties from the specific geometrical arrangement of multiple individual units, known generally as periodic unit cells, rather than from their chemical composition. In fact, it is the specific size, shape, geometry, orientation and arrangement of these elements that determines how the metamaterial interacts with, for example, light or sound.

**NERI’s phononic crystals project**
Under the umbrella of Delft’s interdisciplinary Nano Engineering Research Initiative (NERI), Aragón is supervising a project to design phononic crystals – metamaterials that are engineered to interact with elastic waves for advanced sensing applications. This is an area of great interest because of the potential applications of phononic crystals for energy harvesting, thermal barriers, elastic and acoustic filters, improved transducers and waveguides. Says Aragón: “That’s why I like to do this line of research. I create new methods that are truly unique, but it’s also really important to me to see these methods being applied to solving challenging problems in industry.”

Mode I opening of a cracked cube. What is remarkable about this simulation is that the crack was placed completely independently from the finite element mesh used: the latter was a simple structured mesh. So in order to see the displacement some post-processing is needed. This was carried out using Aragón’s Discontinuity-Enriched Finite Element Method.