Deep Learning Applications in the NanoSolveIT cloud platform: Predicting the effects of exposure to nanomaterials on Daphnia Magna

National Technical University of Athens
UNIVERSITY OF BIRMINGHAM
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NovaMechanics

Pantelis Karatzas[1], Georgia Melagraki[2], Laura-Jayne A. Ellis[3], Iseult Lynch[3], Dimitra-Danai Varsou[1,2], Antreas Afantitis[2], Andreas Tsoumanis[2], Philip Doganis[1], Haralambos Sarimveis[1]

1 School of Chemical Engineering, National Technical University of Athens, Athens, Greece. 2. Nanoinformatics Department, NovaMechanics Ltd, Nicosia, Cyprus 3. School of Geography, Earth and Environmental Sciences, University of Birmingham, Birmingham, United Kingdom

Overview

- A multigeneration study on D. magna exposed to freshly dispersed and aged ENMs of various concentrations in different media was conducted.
- A computational workflow based on AI and deep learning methodologies has been developed with the ultimate goal to assess the type and the severity of malformations compared to the control.
- The proposed models can reduce time-consuming procedures needed for image classification by human experts through automation and thus accelerate hazard assessment and facilitate the development of safe-by-design ENMs.

Introduction

Design of safe engineered nanomaterials (ENMs) is an important challenge in the field of nanotechnology , because due to their small size, ENMs may result in the modulation of pathways and mechanisms of toxic action that may endanger human health and the environment. Several nanoinformatics approaches, including nanoQSAR modelling, read-across predictions and image analysis techniques have been developed to address this challenge with the goal of reducing to the greatest possible extent the need for traditional hazard and risk assessment methodologies which are based on animal testing. Deep learning is a relatively new discipline in the field of machine learning, which proves to be very efficient in analysing big data, with particular emphasis on large sets of images. Given that the collection of experimental data regarding the safety of ENMs is rapidly increasing, deep learning offers excellent methodologies for analysing and modelling these data. This work summarises the key finding and outcomes of the first application of deep learning methodologies on the analysis of electronic images, which are relative to the safety of ENMs (P. Karatzas, G. Melagraki, L-J. A. Ellis, I. Lynch, D-D. Varsou, A. Afantitis, A. Tsoumanis, P. Doganis, H. Sarimveis, *Development of Deep Learning Models for Predicting the Effects of Exposure to Engineered Nanomaterials on Daphnia magna*, Small, 2020, 2001080).

Methods

This work builds upon one of the most extensive ecotoxicological datasets available consisting of more than 4000 electronic images of Daphnia Magna, and combines several deep learning technologies to develop a computational workflow, which addresses the problem of identifying the effects of exposure to coated or uncoated TiO2, Ag or AgS ENMs in different experimental conditions. The workflow (Figure 1) starts with detecting seven regions of interest (Head, Eye, Heart, Abdomen/Claw, Tail, Tail-tip, Tail-base) and continues with computing the overall size and the tail length. Cropped images of the abdomen/claw and heart regions are used as inputs to specially trained deep learning models to classify them with respect to lipid concentrations. The results are compared to control images to determine the types and levels of malformation. The Single Shot Detector (SSD) mobile net v1 and the Residual Convolutional Neural Network (CNN) architectures were selected as the most efficient methods for object detection and image classification problems, respectively. Transfer learning was employed to accelerate the process of training the deep learning models.

Results

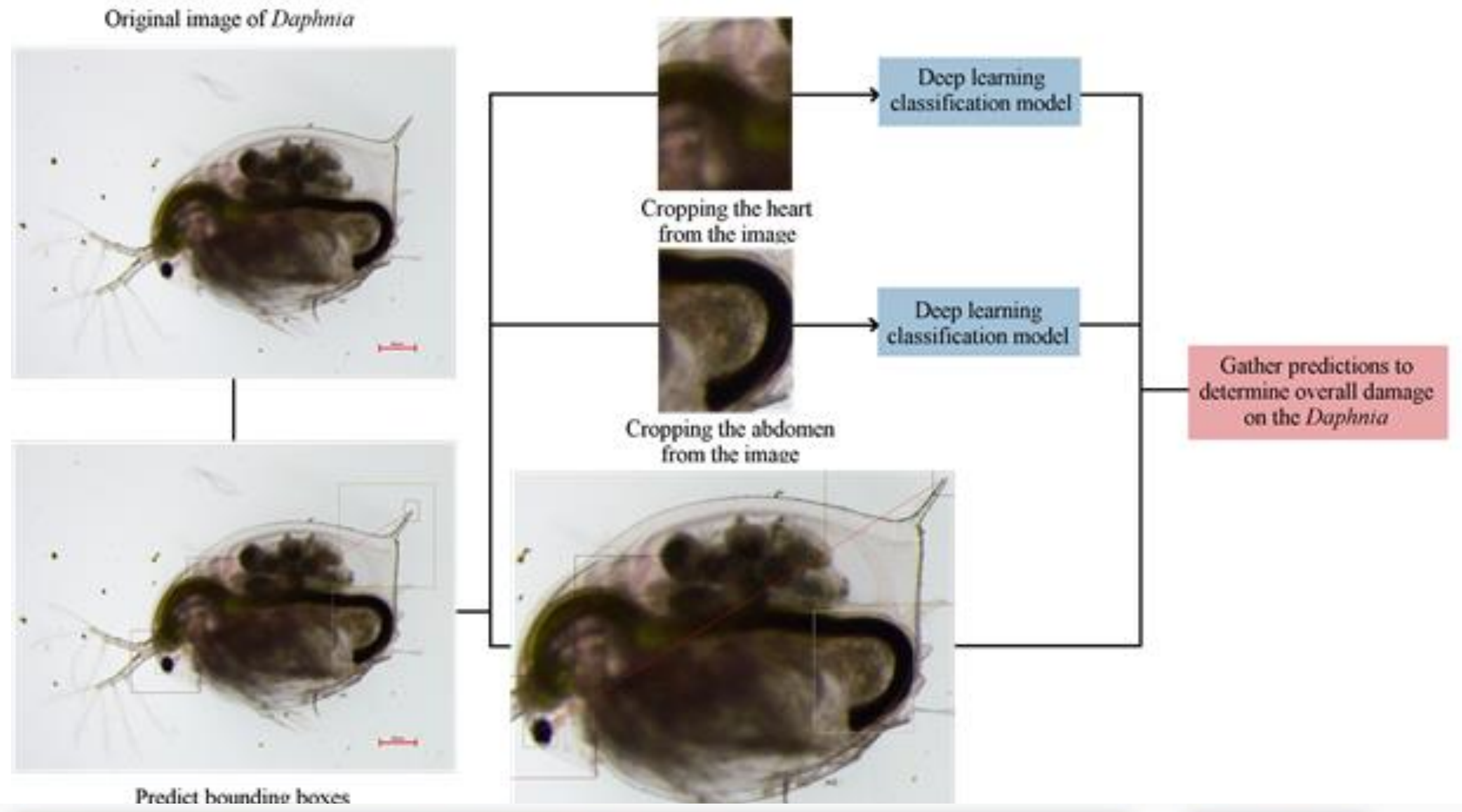

Figure 1.

A graphical representation of the workflow used in the deep learning analysis

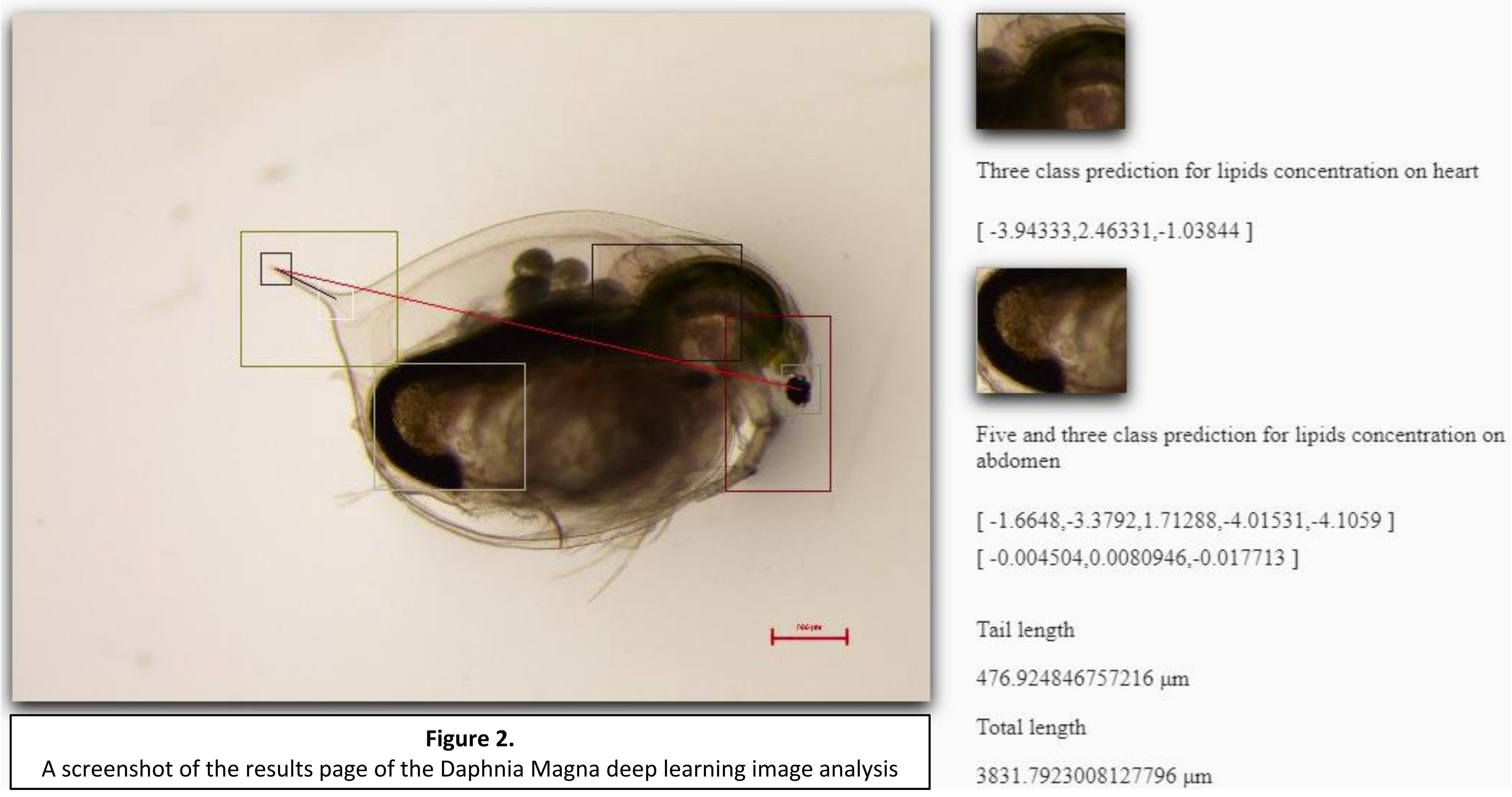

Figure 2.
A screenshot of the results page of the Daphnia Magna deep learning image analysis

The available set of images was partitioned into training and test sets, which allowed an extensive and exhaustive validation of the deep learning models. The complete workflow has been integrated into the NanoSolveIT cloud platform as a user-friendly web application, which is accessible through the following link: https://deepdaph.cloud.nanosolveit.eu/. Here the user just needs to upload an electronic image of a Daphnia Magna exposed to ENMs and the complete workflow is executed automatically.

The result page (Figure 2) contains a copy of the electronic image where the seven regions of interest are indicated in coloured boxes, measurements of the overall size and the tail length, cropped abdomen and heart images and the lipid concentration predictions of the classification models. The same workflow can be applied to control images and comparison of the results allows to detect the types and levels of malformations due to exposure to ENMs. The produced web application is freely available to the community and illustrates that deep learning models and workflows can substitute and optimise time- consuming human-based image classification procedures, accelerate hazard assessment and eventually facilitate the development of safe-by-design ENMs.

Conclusions

A computational workflow based on AI and deep learning methodologies has been developed to first detect, isolate, and classify regions of interest on the Daphnia images where specific malformation occurs and then to assess the type and the severity of malformations compared to the control.

To the best of our knowledge, this in silico study is the first attempt reported to develop validated deep learning predictive models to an extensive ecotoxicological study for predicting the effects of the direct or parental exposure to ENMs on Daphnia. The proposed models can automate time-consuming procedures needed for image classification by human experts and thus accelerate hazard assessment and facilitate the development of safe-by-design ENMs.

Future work will involve extensions to allow adverse effects prediction for subsequent generations, based on parental exposure images with the aim to reduce the time and cost involved in long-term reproductive toxicity assays over multiple generations.

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