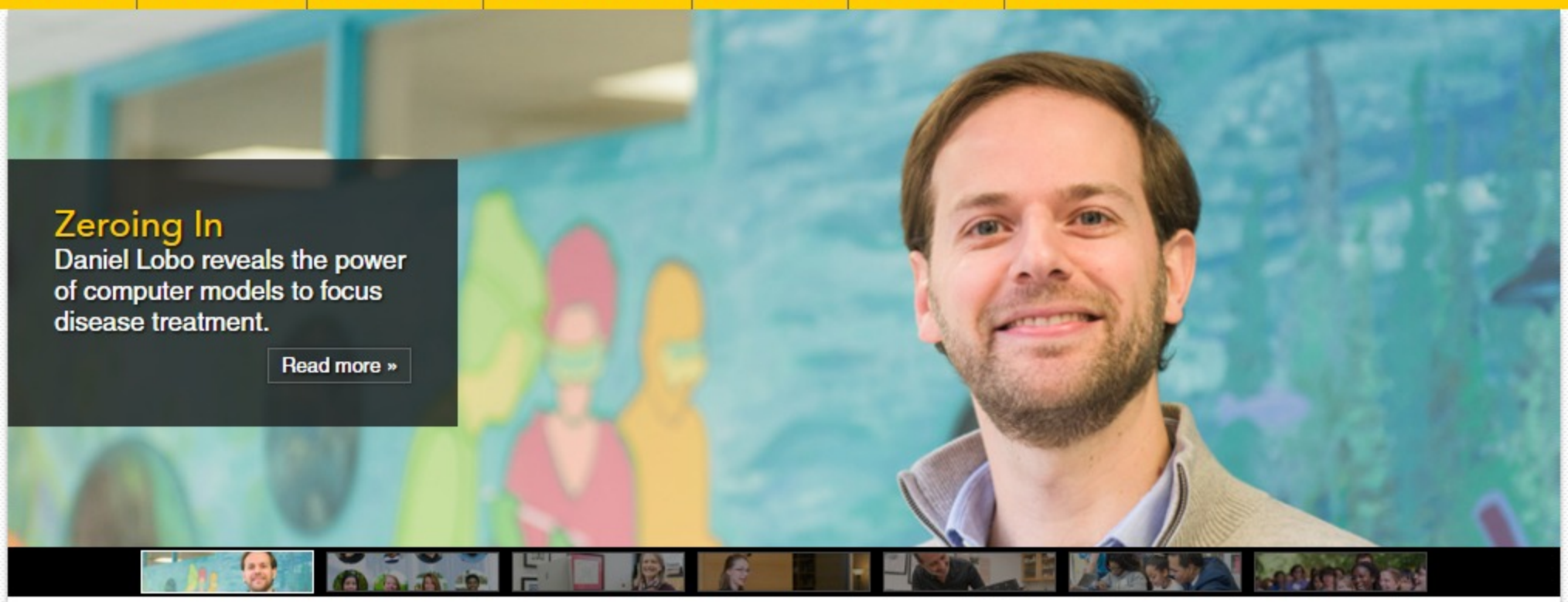

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Daniel Lobo's research reveals power of computer models in disease treatment

Daniel Lobo has a knack for using artificial intelligence to solve biological puzzles, and his latest scientific paper is proof of concept that computer simulations can predict never-before-seen biological outcomes. The **new article** in *Scientific Reports* focuses on a model Lobo, assistant professor of biological sciences at UMBC, developed in collaboration with Michael Levin's lab at the **Allen Discovery Center** at Tufts University.

Lobo's model examines the development of pigment cells in frog embryos. He codified dozens of experiments on tadpole development and input the data into his program, which then "learned" how different drugs and proteins affect the growth of pigment cells in the frog. The model the computer discovered explained how certain combinations of treatments could induce cancer-like cell behaviors in tadpoles. Lobo envisions using the same process of teaching a computer to understand complex drug effects to predict, for example, the most effective drug treatment plans for individual cancer patients.

In the experiments, tadpoles either developed normally or were completely covered with invading pigment cells that had converted to a cancer-like state; there were no tadpoles with a mix of cancer-like and normal pigment cells. To test the predictive power of his model, Lobo wanted to determine if he could use it to find a combination of drugs that could generate a different outcome: an "in-between" tadpole, with some normal and some cancer-like pigment cells. Among 576 simulated experiments, the program identified only one specific combination of treatments that it predicted would produce that result.

Levin and Maria Lobikin, a past member of Levin's lab, collaborated on the new paper to test the model's prediction with real tadpoles, and it proved to be correct. Frog embryos given the specific cocktail that Lobo's program identified (two drugs and a specific small strand of genetic material called an mRNA) developed into tadpoles that contained both normal areas without pigment cells and areas covered with invading cancer-like pigment cells.

Using traditional methods to identify the drug cocktail would have been much more costly and laborious, if it were possible at all. And it would have required a huge number of frog embryos and experiments. Alternatively, explains Lobo, "You can do a lot of cheap experiments inside a computer." Plus, he says, "It only uses virtual frogs."

Lobo hopes the method he used to create his new model can be put to work to find more effective treatments for human diseases, and his first target is cancer. The first—and by far most challenging—step is to generate a program with artificial intelligence that can learn from the data in published studies to create a model for the disease. Lobo's lab is in the early stages of that process with cancer.

Once his program has used the data to generate a model, predicting a desired outcome should be straightforward, says Lobo. "You can simulate any drug, any intervention," and in any combination, he explains, as long as the effects of any single intervention are understood. The ultimate goal, Lobo says, "is to find the best intervention or combination of interventions to get the person back to a normal state."

His work may have started with frogs, but Lobo believes the predictive power of computer simulations has the potential to revolutionize human disease research and treatment. Focusing more intensive research on the specific interventions that computer simulations predict will be most effective would dramatically speed up the timeline for getting patients treatments that work.

Using artificial intelligence this way might also enable "very targeted, personalized medicine," says Lobo. With human patients, doctors don't have the luxury of hundreds of trials. "You may only have one chance, and it may be life or death," he says. "You want to be sure the first treatment has the best chance of curing the disease."

*Read **"Discovering novel phenotypes with automatically inferred dynamic models: a partial melanocyte conversion in Xenopus"** in* Scientific Reports.

Image: Daniel Lobo at UMBC. Photo by Marlayna Demond '11 for UMBC.

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