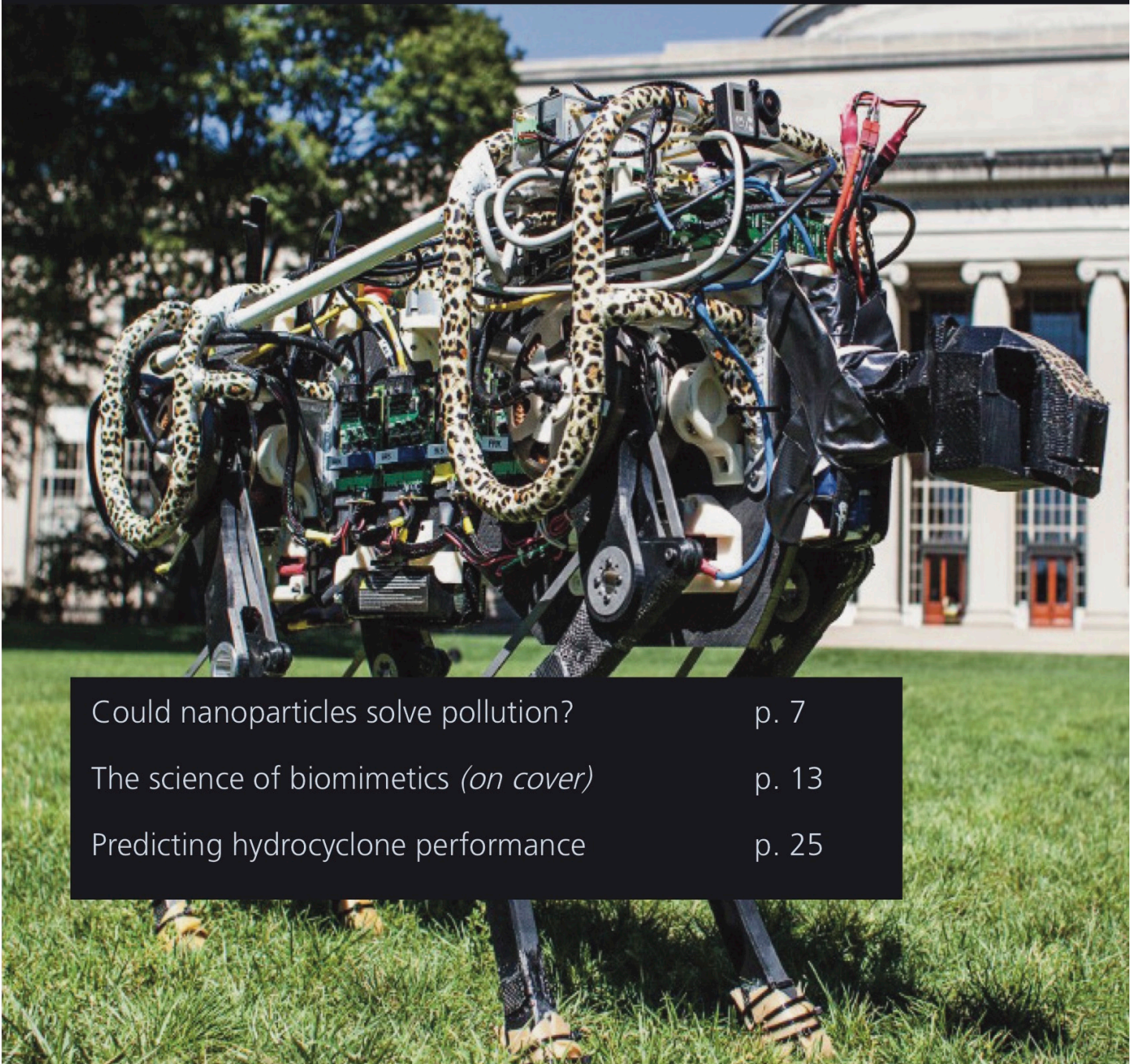


Volume 30 Fall 2015

# MURJ

Massachusetts Institute of Technology  
Undergraduate Research Journal



Could nanoparticles solve pollution?

p. 7

The science of biomimetics (*on cover*)

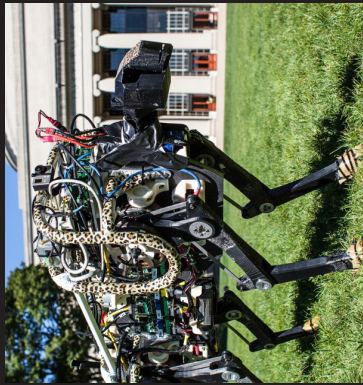
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Predicting hydrocyclone performance

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# MURJ

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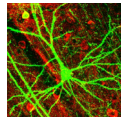
From Tyler Jacks  
From MURJ Editors



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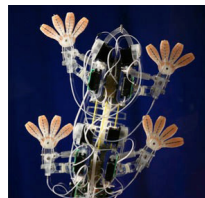
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A look at the latest MIT Science News.



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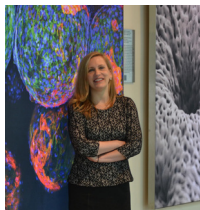
### Features



**Built by Humans,  
Designed by Nature**

*Recreating spider silk, imitating shark skin for swimsuits, even creating a robot inspired by the Earth's fastest animal- this all is involved with the science of biomimetics, the growing field in which designs from nature are taken and applied to solve humans' most complex problems.*

**12-15**



**MURJ Spotlight:  
Dr. Angela Koehler**

*Principle Investigator,  
Koehler Lab @ MIT*

*This issue's spotlight features Dr. Angela Koehler, the Principle Investigator of the Koehler Lab @ MIT and an Intramural Faculty member at the Koch Institute for Integrative Cancer Research.*

**16-20**

## Research Reports

### Impact of Neutron Resonance Elastic Scattering Energy Intervals on Nuclear Reactor Reactivity Calculations

Vivian Y. Tran, Jonathan A. Walsh, Benoit Forget, Kord Smith

*This study explores the impact of resonance elastic scattering on nuclear reactivity calculations through various treatments of the phenomenon in the OpenMC particle transport code. The results come from fresh fuel pin cell benchmark simulations, based on a BEAVRS-verified model of an operating light water reactor. The  $k$ -eigenvalues calculated from DBRC and ARES, two different but accurate treatments of resonant nuclides, are shown to be in excellent agreement (within 2 standard deviations). By applying the corrections only to the necessary energy intervals, a significant improvement in runtime can be achieved...*

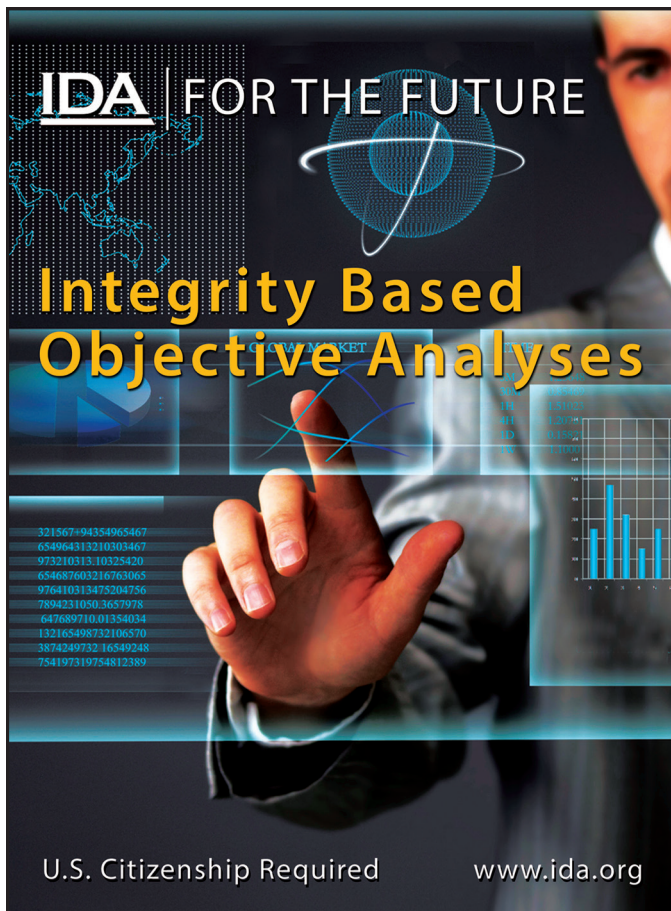
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### Creation of a Model to Predict Plant Hydrocyclone Performance Using Computational Fluid Dynamics

Isaac A Cabrera, Koichi Momono, Ryota Murai

*This report highlights the creation of a simulation model in ANSYS FLUENT™ to predict the separation performance of a plant hydrocyclone. The complex three-phase flow within the hydrocyclone was carefully addressed using various methodologies. The internal flow field was initialized using the Reynolds stress turbulence model and the air core was generated using the Volume of Fluid multiphase model; particle interactions with the continuous phase were resolved using the Eulerian-Lagrangian particle tracking method and one-way coupling. The flow split and particle collection efficiency were then compared to existing industrial data...*

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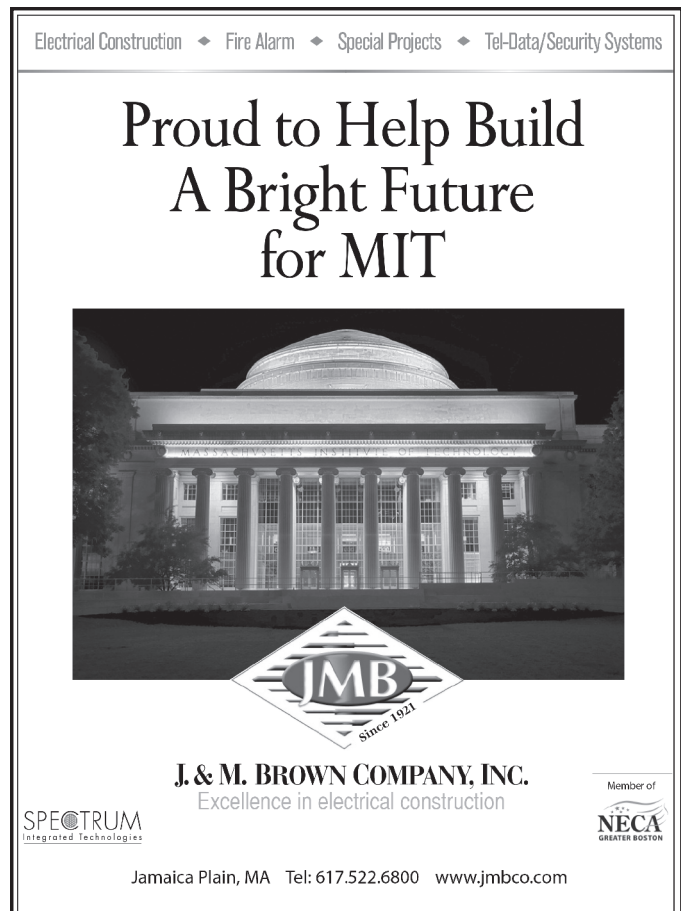


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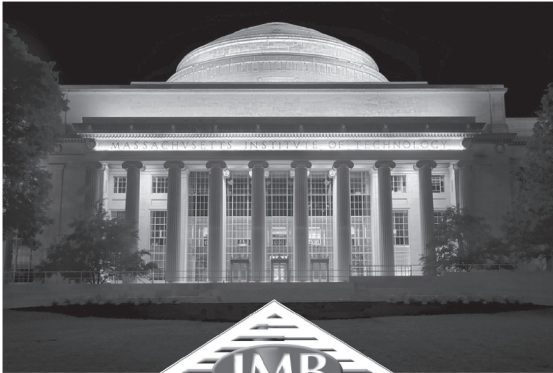
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**Tyler Jacks**

Director, Koch Institute for Integrative  
Cancer Research at MIT

**Massachusetts Institute of Technology**

77 Massachusetts Avenue  
Cambridge, Massachusetts 02139-4307

December 2015

Dear MIT Community,

I am pleased to be able to introduce the Fall 2015 issue of the MIT Undergraduate Research Journal (MURJ). MURJ is a written symbol of one of the core strengths of an MIT undergraduate education: the ability to conduct cutting-edge research at one of the world's leading research universities. In laboratories across our campus and in all of the fields of study that we pursue, undergraduates are working to advance knowledge and to develop new technologies. The articles published in this issue represent the high quality of research in which our students are engaged. Collectively, our undergraduate researchers make major contributions to all that we do at MIT.



Since my arrival at MIT as a post-doctoral researcher in the laboratory of Robert Weinberg in the Whitehead Institute and over the past 23 years on the faculty, I have trained more than 100 undergraduates through the Undergraduate Research Opportunities Program (UROP). These students have helped move our research into the genetics of cancer significantly forward, and they have also helped their graduate student and post-doctoral mentors learn the skills of supervising and motivating junior colleagues. They have experienced the excitement of discovery as well as the many challenges that must be overcome to make progress. It has been a genuine thrill for me to witness so many of these students catch the research bug and head off from MIT to pursue advanced degrees in science. Others have taken their talents to medical school or other professional pursuits, but I am confident that all of them have a much greater appreciation of what it is to do research thanks to their time in the lab.

MIT's highly interdisciplinary approach to research is also reflected in the UROP experience as well as in MURJ. Our students blur the lines between disciplines and help to create altogether new ones. In a world that needs novel solutions to long-standing problems—from cancer to climate change—the bright young minds of our undergraduate researchers are a wonderful source of creativity and innovation. I have no doubt that as a group, MIT's UROP students are the most talented undergraduate research workforce in the world.

I hope you enjoy this issue of MURJ. It is the product of a great deal of hard work and commitment from a very special group of students. They do us proud.

A handwritten signature in black ink, appearing to be "TJacks".

Sincerely,  
Tyler Jacks

Director, Koch Institute for Integrative Cancer Research at MIT  
David H. Koch Professor of Biology  
Investigator, Howard Hughes Medical Institute



**UNDERGRADUATE  
RESEARCH JOURNAL**  
Volume 30, Fall 2015

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MIT Undergraduate Research Journal



**Massachusetts Institute  
of Technology**

December 2015

Dear MIT community,

We are excited to present to you the 30th issue of the MIT Undergraduate Research Journal (MURJ), a biannual student-run publication featuring exemplary undergraduate research at the Institute. For 15 years, MURJ has provided a platform for undergraduates to showcase their passion for scholarly pursuits across a variety of disciplines. We are amazed by the professional quality and brilliance of the research reports published in this issue. Research presented here involving the use of computational fluid dynamics to predict performance of a plant hydrocyclone is an example of collaboration with the Institute and a global Japanese company and also exemplifies the Institute's emphasis on interdisciplinary work. Another research report from the Department of Nuclear Science and Engineering once again represents the meaningful impact a student's work can have on an academic field. Proud of the thrilling and motivated research at the Institute, we are honored to share these students' work with the MIT community.

In addition to our research reports, we highlight current science news articles and present feature articles elaborating on interesting discoveries and interviewing prominent scientists and engineers around the Institute. In this issue, we looked at the study of biomimetics, where designs in nature are studied and applied to solve problems in engineering and science. We also sat down with MIT Assistant Professor of Biological Engineering, Angela Koehler, to discuss her career path, teaching and mentorship, and thoughts on the future of biological engineering.

We hope that this journal is a representation of how highly students value complementing their education with hands-on

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Massachusetts Institute  
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MURJ Staff  
MIT Undergraduate Research Journal

research in world-class laboratories that the Institute provides great resources for. The intellectual curiosity that fills this journal is an extension of the innovative spirit that is prevalent throughout the Institute. This issue has been made possible by a collaborative team of dedicated students, faculty, and departments. We would like to thank the student researchers who shared their research here and the MURJ staff members for their work this semester, without which this issue would not be possible.

For previous issues of the MIT Undergraduate Research Journal, visit our renovated website at [murj.mit.edu](http://murj.mit.edu). If you are interested in submitting work or joining our team for future issues, we invite you to contact us at [murj-officers@mit.edu](mailto:murj-officers@mit.edu).

Best,

Tatyana Gubin  
(Co-Editor-in-Chief)

Linda Jiang  
(Co-Editor-in-Chief)

Lakshmi Subbaraj  
(Co-Editor-in-Chief)

Massachusetts  
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Volume 30, Fall 2015

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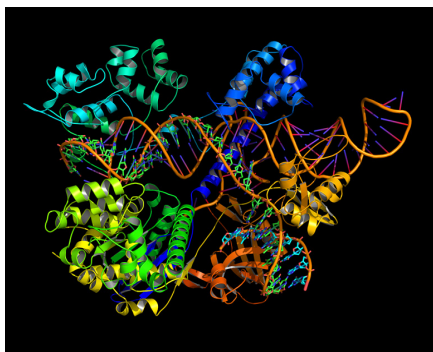
# MIT Science News In Review

## GENETIC ENGINEERING

### MIT Scientists Discover New Genome Editing System

Ever since its discovery, CRISPR-Cas9 has had a monumental impact on the field of molecular biology and genetic engineering. This genome-editing tool, which is derived from the adaptive immune system of *Streptococcus pyogenes*, allows researchers to introduce site-directed double stranded breaks in DNA in order to either silence a gene or insert a desired DNA sequence. Due to its specificity, low cost, and efficiency, CRISPR-cas9 has proven to be an invaluable tool in the modeling of diseases and the development of new therapeutic treatments.

Considering the many applications of CRISPR-Cas9, Feng Zhang, a W.M. Keck Assistant Professor in Biomedical Engineering in MIT's Department of Brain and Cognitive Sciences, wondered if there were other CRISPR systems in nature that could also be used as tools for genome editing. In a paper published in *Cell*, Zhang and his colleagues characterized CRISPR-



**Crystal Structure *Staphylococcus aureus* Cas9 complex form.**

Credit: <https://www.broadinstitute.org/blog/zhang-lab-unlocks-crystal-structure-new-crisprcas9-genome-editing-tool>



*Training object-recognition systems involves feeding photos like the one above into a computer along with one expected result (i.e. "beach"). If the algorithm output did not match the expected result (i.e. "sand" instead of "beach"), it would be retrained. However, MIT CSAIL's new training system improves accuracy by rewarding guesses that are semantically similar to the expected result (such as "sand" instead of "beach").*

Credit: [https://upload.wikimedia.org/wikipedia/commons/9/96/Beach\\_pano.jpg](https://upload.wikimedia.org/wikipedia/commons/9/96/Beach_pano.jpg)

Cpf1, a previously unstudied CRISPR system derived from the bacterial species *Acidaminococcus* and *Lachnospiraceae*. CRISPR-Cpf1 differs from the CRISPR-Cas9 in several important ways. It requires only one gRNA, compared to the two employed by Cas9, to direct the Cpf1 enzyme to the desired editing site; while Cas9 cuts both strands of DNA at a time, leaving "blunt ends" that often undergo mutations as they are rejoined, Cpf1 facilitates more precise insertion by leaving short overhangs when it makes a cut; and unlike Cas9, Cpf1 cuts far away from the recognition site, allowing for correct editing to occur even if the gene becomes mutated at the cut side. Finally, Cpf1 provides new flexibility in choosing an editing site, since it recognizes very different "PAM" sequences—short DNA sequences following the target, and required for binding—than Cas9. Zhang and his colleagues showed that this new CRISPR system, like CRISPR-Cas9, has the ability to edit a human genome, and thus possesses powerful applications in various fields. They aim

to make the CRISPR-Cpf1 technology widely accessible, with the Broad Institute and MIT providing licenses to other labs so that they too can add the Cpf1 enzyme to their repertoire. CRISPR-Cpf1 will undoubtedly become an useful tool in the field of molecular biology, and is one of many examples of how MIT has been in the vanguard of genomics.

—S. Santiago

Source:

<http://news.mit.edu/2015/crispr-editing-dna-genome-engineering-0925>

## MACHINE LEARNING

### Improved Machine Learning from More Qualitative Training

A team of MIT researchers have created a new method in machine learning by which related concepts are utilized to reinforce one another. The team of researchers consisted of Tomaso Poggio, a Eugene McDermott Professor in the Department of Brain and Cognitive Sciences and at the Artificial Intelligence Laboratory, graduate students Chiyuan Zhang

and Charlie Frogner, postdocs in the Computer Science and Artificial Intelligence Laboratory, and Shell Oil researcher Mauricio Araya-Polo.

Object-recognition algorithms generally utilize probabilistic means of determining the identity of an object in a given image. For instance, an algorithm may suggest with a certain probability that an image is portraying a woman and with another probability that the image is portraying a man. Based on the greater probability, the algorithm then predicts the identity of the object in question. The MIT team's new algorithm, however, will allow for the reinforcement of classifications. For example, in the case of human recognition more weight would be placed on an

image's classification as "man" and "boy" together rather than "man" and "woman" together.

Typically, machine learning algorithms used by websites such as Flickr will predict potential tags by identifying key features of images and matching them to tags often used in similar images. Using this form of training, the program would be "penalized" for every incorrect tag and "rewarded" for every correct tag.

In contrast, the MIT team's new algorithm rewards "partial credit" for incorrect tags that are similar to the correct tag. For example, the traditional method would penalize an image of a tree that was classified as "leaf" and "nature" the same as if

it were classified as "leaf" and "building". The new method, however, provides a partial reward for the correctness of a tag semantically similar to the image and thus increases the likelihood that, for example, the tags "leaf" and "nature" co-occur in the future. As Zhang explained, "Because there are actually semantic similarities between those categories, we develop a way of making use of that semantic similarity to sort of borrow data from close categories to train the model."

The researchers found that when their algorithm was used to classify images on Flickr, their method of training was able to predict the tags placed on the image by Flickr users

## ENVIRONMENTAL SCIENCE

### Nanoparticles Have Potential to Cleanup Environmental Pollutants

A "happy accident" led a team of researchers from MIT and the Federal University of Goiás in Brazil to discover a potential new use for nanoparticles: the quick isolation and elimination of human-made environmental pollutants. Ferdinand Brandl and Nicolas Bertrand, former postdocs in the laboratory of MIT Professor Robert Langer, were initially working to develop nanoparticles that could be used to deliver cancer drugs when they realized their potential in environmental remediation.

At first Bertrand and Brandl sought to use nanoparticles previously synthesized by Brandl, which converted to macroscopic aggregates upon exposure to ultraviolet (UV) light, as vectors for drug delivery. They came to abandon this line of inquiry, however, since UV light can be damaging to tissue, and does not penetrate well through the skin. Learning that some water treatment facilities use UV light as a disinfectant, they began to consider another use for the particles: combining their ability to form aggregates with the pathogen-eliminating ability of UV light in order to provide an effective



**Nanoparticles optimized for drug delivery could be used to effectively remove a variety of environmental pollutants.**

Credit: [https://commons.wikimedia.org/wiki/File:Spechtensee\\_gegen\\_Nordosten\\_01.JPG](https://commons.wikimedia.org/wiki/File:Spechtensee_gegen_Nordosten_01.JPG)

new method of pollutant removal. They synthesized environmentally friendly nanoparticles from polyethylene glycol, an FDA-approved food additive, and polyactic acid, a biodegradable plastic. Enclosed by a hydrophilic shell, the particles dissolve readily into water; upon irradiation with UV light, however, their outer shell is shed, revealing a hydrophobic inner core. Removal of the stabilizing outer shell causes the particles to form macroscopic aggregates containing absorbed

hydrophobic pollutants, which can be easily removed by filtering or sedimentation.

The team's preliminary experiments suggest that their treatment method can significantly reduce the teratogenicity—or ability of a chemical to cause abnormalities in physiological development—of BPA, triclosan, and 17 $\alpha$ -ethinyl estradiol, all three of which are introduced to the environment in high concentrations by human activity. BPA is an organic synthetic compound commonly used to manufacture plastics, while triclosan is an antibacterial found in soaps and detergents, and 17 $\alpha$ -ethinyl estradiol is the main component of estrogen-based oral contraceptive pills. These findings not only indicate the broad applicability of the team's synthesized particles, but suggest the larger potential of adapting nanoscale drug delivery techniques to environmental remediation.

—J. Switzer

Sources: <http://news.mit.edu/2015/nanoparticles-clean-environmental-pollutants-0721>  
Brandl, F. et al. Nanoparticles with photoinduced precipitation for the extraction of pollutants from water and soil. *Nat. Commun.* 6:7765 doi: 10.1038/ncomms8765 (2015)

more accurately than traditional training methods.

The main obstacle posed by this “partial credit” method is the increased complication of calculating the scores of predictions. For instance, while the traditional method simply scores the resulting tags as “true” or “false”, this new method, needs to vary its calculations to take into account the various scenarios in which some of the tags are right and the others are wrong. To cope with this complication, the researchers made use of the Wasserstein metric (a method of comparing probability distributions) as an error metric. Without this error metric, the computation would not be efficient. The researchers believe that their paper is the first use of the Wasserstein distance in machine learning where the system’s performance is compared to human classifications.

This machine learning method will be presented this December at the Annual Conference on Neural Information Processing Systems.

—R. Waldman

Source: <http://news.mit.edu/2015/more-flexible-machine-learning-1001>

## LINGUISTICS

### Demystifying Language Acquisition

All human languages consist of phonemes, the basic sonic components that construct words. Phoneme acquisition in infants and children remains a mystery, but Chia-ying Lee, Timothy O’Donnell and James Glass of the Computer Science and Artificial Intelligence Laboratory have developed a possible model to study this phenomenon. This model is unique in that it requires no human mediation to distinguish between phonemes or words. Rather than requiring humans to create a dictionary of sounds, it is able to compile its own library of language. It categorizes language into three hierarchical cat-



**Researchers at the Computer Science and Artificial Intelligence Laboratory created a model to elucidate how the developing brain acquires language.**

Credit: Public Domain

egories: word-like, sub-word-like, and phoneme units.

The model synthesizes various analytic methods in order to learn these linguistic structures. Among these are adaptor grammar, noisy-channel, and acoustic models. Adaptor grammars parse speech using probability, while noisy-channel models account for differences among spoken speech by assuming that any audio is a distorted set of true phonemes. The acoustic model determines the length of various phonetic units.

Various MIT lectures were fed into the model, which combed through the audio to collect linguistic units. It was largely successful in identifying words and phonemes, but often categorized repeated phrases such as “open university” in an Economics lecture as single words. This is likely due to the relatively small variation in word usage the model analyzed — it was only privy to academic lectures on certain topics.

Nonetheless, the new system has promise in deciphering language

development in humans. Lee, O’Donnell and Glass hope to further develop this system as well as search for more effective alternatives to detect variance in human speech.

—N. Syed

Source: <http://news.mit.edu/2015/learning-spoken-language-phoneme-data-0914>

### Shorter is Sweeter

The rich diversity of human language intrigues many, and finding similarities among the body of languages can lend important information as to the variation of languages and the function of the brain itself. Richard Futrell, Kyle Mahowald, and Edward Gibson at the TED Lab in the Department of Brain and Cognitive Sciences studied 37 languages and observed that most optimize the distance between vital components of sentences. For instance, to an English speaker, the sentence “Sarah picked up the cake from the bakery,” sounds more natural than “Sarah picked the cake up from the bakery.” In the second

sentence, there are several words between “picked” and “up.” This distance is known as “dependency length,” since the meaning of the





**Social networks on a national scale are geographically determined and tend to cluster around urban areas.**

*Credit: Copyright free, public domain*

studied how connected components emerge within cities, and their relation to physical space. Using information from 7 billion mobile phone interactions gathered within a 6 month period in France, Portugal, and Spain, they determined the geographic distance between users by assigning to each person a single location corresponding to their most commonly used zip code. The social distance between two people was determined by the number of people in the smallest “social group” that contained them both. These social groups were determined using the Newman Girvan modularity network, which detects social groups, or “network communities,” by successively removing social connections that are likely between—rather than within—communities.

After mapping out their measured networks, the researchers used them to test the performance of different routing strategies, or methods of choosing paths within a network, at finding a particular target within a city. They found that “geogreedy” strategies, which choose routes based on the smallest geographic distance to their target, were ineffective, while strategies that choose routes based on smaller

social networks were successful. On a national scale these “geogreedy” algorithms were effective at reaching a target city; however, once within the cities’ borders new algorithms based on social interactions were needed in order to reach the target individual.

“Searchability” is a well-established network property which implies that ordinary people have the ability to direct messages only through their acquaintances and reach any target person in only a few steps. Using email communication, Dodds et al. showed that, in general, people in the first few steps tend to select acquaintances that are geographically close to the target, while in the last steps, acquaintances belonging to the same professional group as the target—and therefore socially close—are selected. The MIT team’s research helps explain why this happens; cities change the structure of social networks, increasing the impact of social proximity on the establishment of network connections.

—J. Switzer

Sources: <http://news.mit.edu/2015/breaking-down-social-networks-cities-0610>

Herrera-Yagüe, C. et al. The anatomy of urban social networks and its implications in the searchability problem. *Sci. Rep.* 5, 10265; doi: 10.1038/srep10265 (2015)

## NEUROSCIENCE

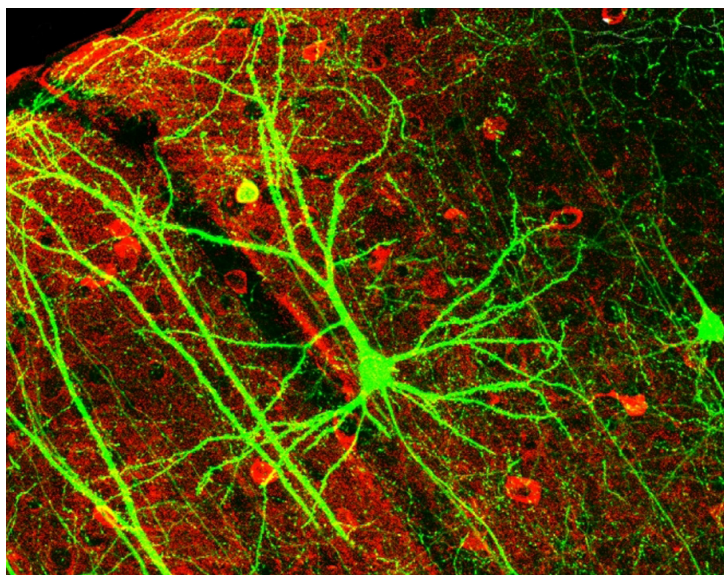
### The Brain’s Time Tracking

A collaboration between researchers at MIT’s McGovern Institute and Columbia University led by Mehrdad Jazayeri, an assistant professor at MIT, has unearthed a mechanism by which the brain tracks and reproduces time intervals.

Their research, published in the Oct. 8 issue of *Current Biology*, describes how the portion of the brain believed to be involved in eye movement—the lateral intraparietal cortex or LIP—also measures time intervals and reproduces their magnitude. Additionally, the pattern of electrical impulses in this region of the brain suggests that it plays a role in the time perception utilized in sensory and motor coordination.

The collaborators conducted their research by analyzing the neural activity in the parietal cortex of monkeys as they performed time reproduction tasks. The monkeys were trained and then tested in exercises in which they recorded time intervals and then reproduced these same intervals. The data collected during these tests demonstrated that the monkeys measured the time interval internally and then translated that into action relative to their desired motor plan to recreate the time period. In these trials, a correlation was found between the phase of measurement and the phase of action. The neuron activity suggests that the end of the monkey’s internal time measurement would directly result in the corresponding signal to match the production of the motor activity. This suggests a direct correlation in time observation and motor response.

Although the LIP appears to be a decisive aspect of the brain’s perception of time, Jazayeri explains that this portion of the brain is only one piece of the mechanism of internal time mea-



**A pyramidal neuron stained with green fluorescent protein.**

Credit: <https://upload.wikimedia.org/wikipedia/commons/d/dc/PLoS Biol.4.e126.Fig6fNeuron.jpg>

surement. According to Jazayeri, his research does not conclude that the parietal cortex is the brain's "timer". More accurately, he describes it as providing "computational principles that explain how neurons' firing rates evolve with time, and how that relates to the animals' behavior in single trials."

Looking forward, Jayzeri's group plans on exploring how measured brain activity changes based on an animal's expectation of a time interval's duration as well as exposure to the same time interval twice before motor reproduction.

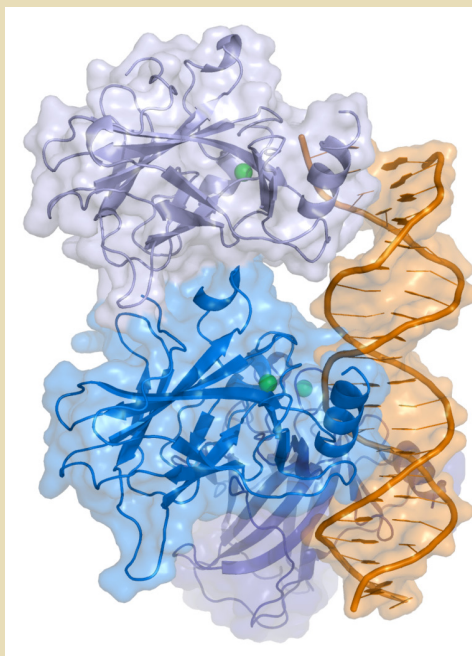
—R. Waldman

Source: <http://news.mit.edu/2015/neuron-firing-patterns-underlie-time-measurement-brain-1008>

## MEDICINE

### Uncovering the Mechanism Behind Resistance to Cancer Drugs

One of the greatest current challenges in cancer treatment is the development of drug resistance. In many patients, a treatment that starts out promising can suddenly become ineffective. Until recently, the mechanism that lead to this drug resistance were not well understood. However, in a recent paper published in *Cancer Cell*, MIT Biology professor Michael Yaffe and his colleagues describe one of the possible pathways cancerous cells can undergo to acquire drug resistance. Yaffe and his colleagues observed that tumors lacking p53, a gene that regulates cell division to prevent harmful DNA mutations, have a backup system, the MK2 pathway, that tells cancer cells to keep dividing even if their DNA has been substantially damaged by chemotherapeutic drugs.



**p53 complexed with DNA.**

Credit: <https://en.wikipedia.org/wiki/P53>

The hnRNPA0 RNA-binding protein plays a key role in this pathway. This protein binds to RNA and triggers changes in the expression levels of certain genes, which in turn lead to uncontrolled cell proliferation. Thus, the hnRNPA0 RNA-binding protein and the MK2 pathway serve as potential drug targets that may provide new alternatives for patients suffering from chemotherapeutic resistance. The researchers found that measuring the RNA levels of genes affected by the RNA binding protein was a good predictor of a patient's response to chemotherapy. The Yaffe lab is now researching and testing new drugs and materials that could be used to target this pathway.

—S. Santiago

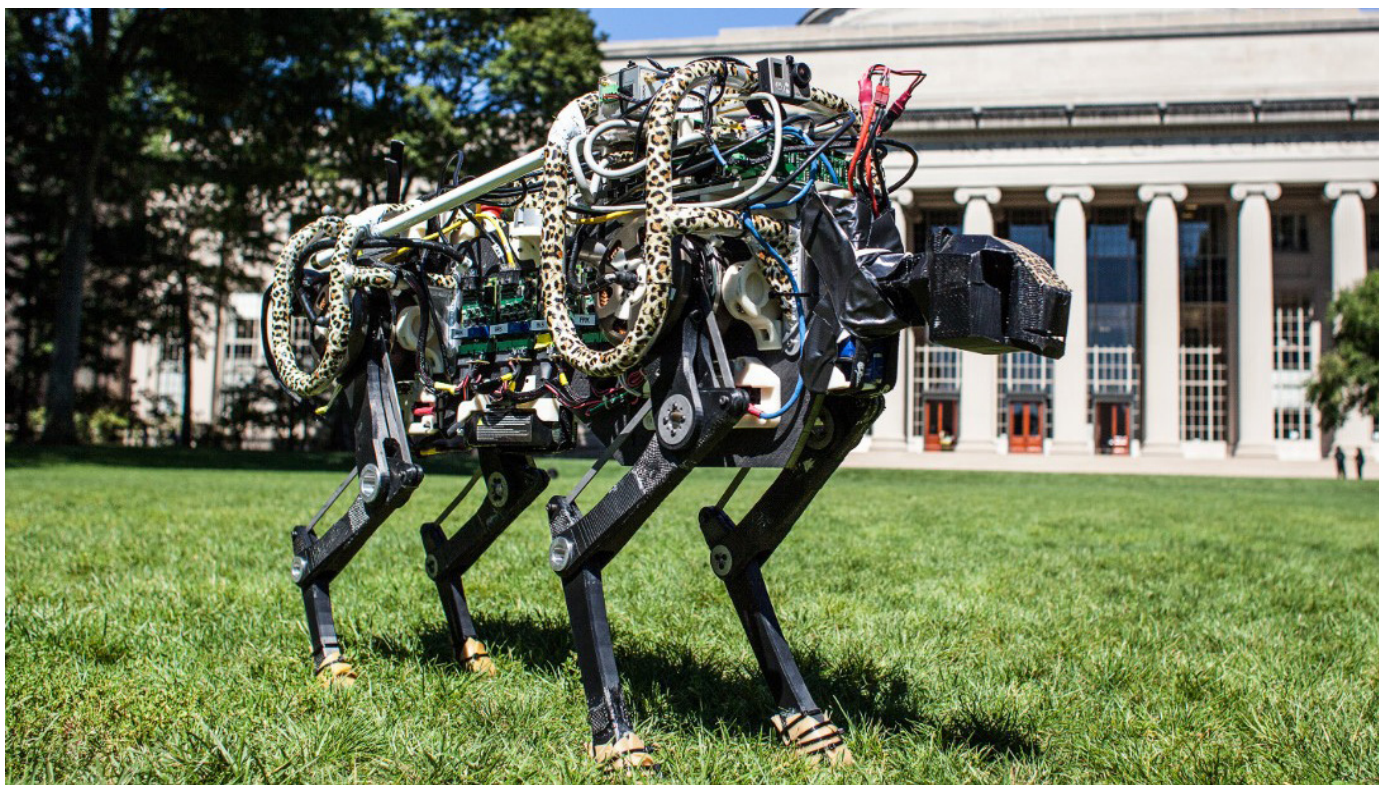
Source: <http://news.mit.edu/2015/finding-drug-resistance-mechanism-tumor-cells-1022>

# MURJ Features

# Built by Humans, Designed by Nature

*Recreating spider silk, imitating shark skin for swimsuits, even creating a robot inspired by the Earth's fastest animal- this all is involved with the science of biomimetics, the growing field in which designs from nature are taken and applied to solve humans' most complex problems.*

BY HELENA MA



***The MIT Biomimetics Robotics Lab built the Cheetah Robot, inspired by the fastest animal on Earth, to potentially use for rescue situations.***

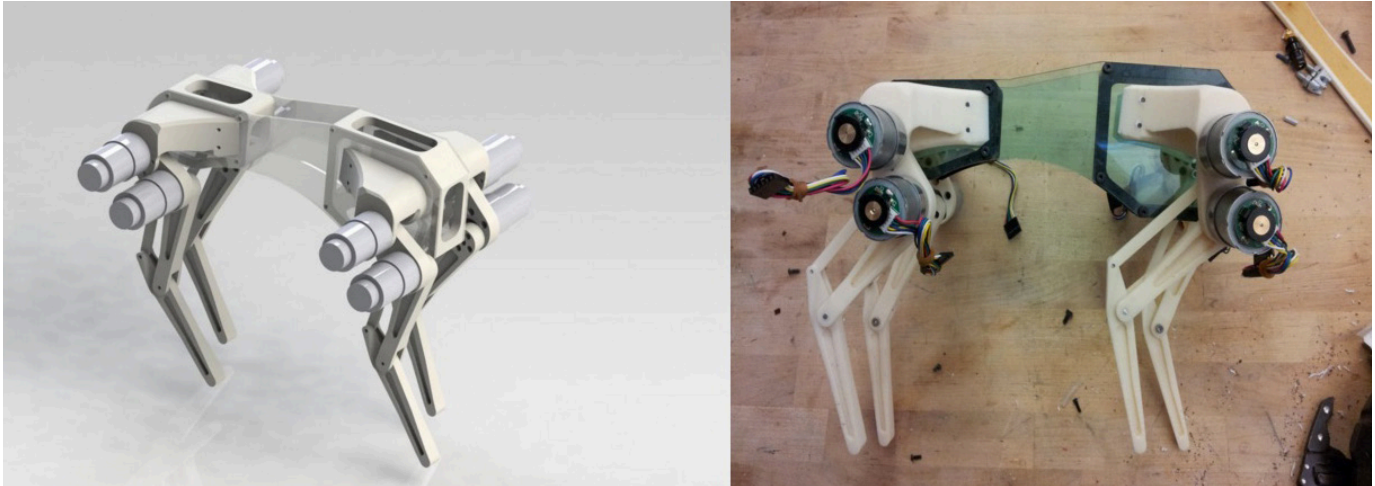
Credit: <http://www.extremetech.com/wp-content/uploads/2014/09/MIT-Cheetah-05-640x366.jpg>

When you use energy from solar panels, look at the bright screen of your cell phone, or put on glittery make up, you may not realize that key components of those technologies are inspired by designs in nature. This idea comprises the study of biomimetics, the imitation of models, systems and elements of nature for solving problems in engineering, material science, medicine, and other fields.

The biomimetics field believes that natural selection and evolution has already solved some of humanity's most complex problems. Scientists and researchers look at these organisms with well-adapted structures and try to imitate them to benefit mankind. Biomimetics has led to new technologies inspired by biological designs from the nano level to the macro level, from solving medical problems

such as environmental exposure tolerance and resistance for humans to engineering problems like harnessing solar energy.

Imagine a rescue mission where someone is in dire need of medical attention yet he's stuck in a dangerous location. Only instead of a person rushing in to help, it's a robot, with a run strikingly like that of a cheetah. That's the image the MIT Biomimetics Lab had in mind



**After the Original Cheetah Robot, the Junior Cheetah was built so further research could be done with a small, inexpensive model.**

Credit: <https://biomimetics.mit.edu/research/mit-junior-cheetah>

when it built the Sprinting Cheetah Robot several years ago, a rapidly-moving robot inspired by the fastest moving animal on Earth. To be able to do further research with a small, inexpensive model, the Junior Cheetah Robot was built by current MIT senior Benjamin Katz during the summer of 2013.

Katz described the usefulness for building the Cheetah Robot.

“The general motivation of the Cheetah was disaster response. Legged robots can go lots of places that things with wheels can’t,” Katz said.

“Humans are incredibly versatile. Right now, there aren’t really many dynamic legged robots. The current robots are really slow, they’re not dynamic and they can’t react

*The biomimetics field believes that natural selection and evolution has already solved some of humanity’s most complex problems.*

quickly. What the Cheetah does, it implements new design techniques that optimize the robot for being really fast.”

Katz said the importance of the biomimetics robotics field is being able to extract nature’s solutions and apply them to robots.

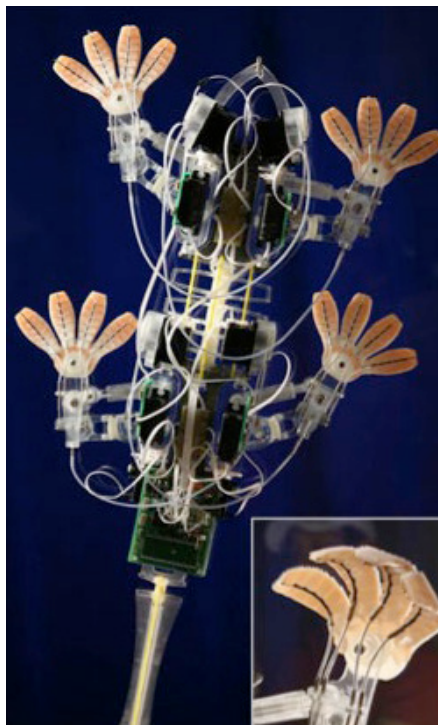
“Animals and humans can do a lot of things that robots can’t do right now. So the point isn’t just to blindly mimic animals, that’s not productive,” Katz said. “The point is to figure out what animals are good at, why they’re good at those things, and extract those principles and apply them to robots. For example, if you look at the Cheetah Robot and compare it to other robots and look at the mechanisms, you notice that the limbs are backdrivable. And that turns out to be really useful. And that’s what allows it to run really fast using electric motors which is something that hasn’t really been done before. It’s an important reason why humans and animals can be dynamic because muscles are backdrivable so that’s one concept taken from nature and used for this robot,” he said.

Researchers and scientists around the world are increasingly turning to biomimetics to find solutions for human problems. According to National Geographic, engineers in England and



**Cockleburs inspired Swiss chemist George de Mestral to create Velcro, which now has mass commercial use.**

Credit: <http://www.discoverlife.org/>



***Inspired by the mechanical properties and geometry of geckos' feet, the Stickychot robot has feet made of directional-adhesive, which allows it to climb.***

*Credit: Sangbae Kim*

Pennsylvania are looking at the the backs of humpback whale to find how to make more agile airplane wings. In Japan, medical researchers are mimicking the tiny serrations on a mosquito's mouth to create hypodermic needles that reduce the pain of an injection. And in Zimbabwe, architects are trying to build more comfortable buildings by studying how termites regulate temperature and airflow in their mounds.

As cool as these biomimetic projects sound, there continues to be a challenge to bring these bio-inspired projects to mass use in the real world. There is arguably only one invention that holds a household name: Velcro. But when it comes to creating artificial spider silk or mimicking gecko adhesion for mass use, scientists have still a bit more to go before it's what they want it to be— despite the

multitude of funding and mass efforts of top scientists.

Part of the explanation for this challenge lies in the fact that biology is just so hard to recreate. Evolution designed a lizard's foot or a whale's back through random experiments over thousands of years, creating organisms whose main goal is to stay alive and produce the next generation of organisms to launch the next round of experiments. Eventually, natural selection would produce organisms that were equipped with the best features possible in order to live. It is difficult for engineers to properly pluck apart all these layers of natural engineering. In addition, the complexity of these organisms' structures requires coordinating joint work among diverse academic and industry disciplines.

For Katz, he spent most of the summer creating the robot to do research, then the actual building took only two weeks at the end of the summer.

"There was a ton of research and thought and prototyping and testing of components that happened the entire summer. The actual building was the last

two weeks of the summer. It was an entire summer's worth of research," he said.

Nevertheless, the gap with nature is slowly closing. Scientists are using powerful technologies to gain insight on nature's microscale secrets, and the growing selection of advanced materials allows them to mimic nature more accurately than ever. While biomimetics is a growing field, it has already become a powerful tool for understanding life.

Katz said he understands the divide between nature's organisms and the projects that engineers are trying to build. But he notes it's not always a bad thing.

"Robots and machines are fundamentally different [from organisms]. They have very different responses and properties and you can't just copy & paste what you see in nature. But sometimes it's a good thing," Katz said. "Sometimes our alternatives are better than nature's alternatives." ■



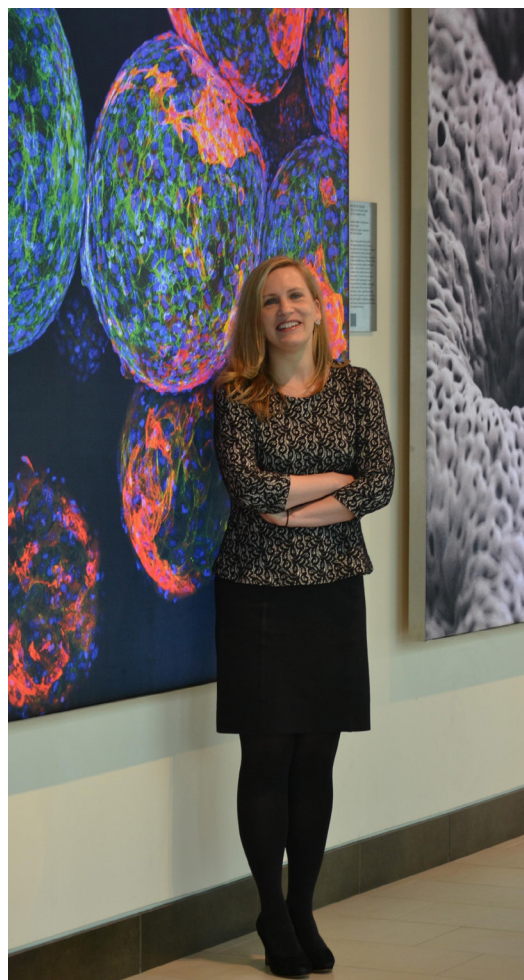
***The Search Serpent Robot mimics the way a snake maneuvers. This high flexibility allows the robot to move through complex environments where people and conventional machinery cannot.***

*Credit: Howie Choset, Carnegie Mellon University*

# MURJ Spotlight: Dr. Angela Koehler

*This issue's spotlight features Dr. Angela Koehler, the Principle Investigator of the Koehler Lab @ MIT and an Intramural Faculty member at the Koch Institute for Integrative Cancer Research.*

BY KIMIA ZIADKHANPOUR



**Dr. Angela Koehler, Principle Investigator of the Koehler Lab at MIT, is building chemical tools and methods that target temporal aspects of transcriptional regulation in development and disease with a focus on cancer.**

*Credit: Koehler Lab archives*

The Koehler Lab @ MIT is building chemical tools and methods that target temporal aspects of transcriptional regulation in development and disease with a focus on cancer. The lab studies these goals by discovering and developing direct small-molecule probes of proteins involved in transcriptional regulation such as transcription factors and chromatin modifying enzymes.

Until very recently, reliable methods were not available for accessing biological systems broadly at their mechanistic levels. Thus, understanding and altering their functional properties was not a realistic possibility. Today, biological engineers can harness the power of innovative technologies to employ them in exciting new ways in the environmental health and other diverse industries.

The lab combines engineering principles and perspective with the knowledge of modern molecular life sciences by developing a general approach to small-molecule probe discovery for transcription factors by coupling direct binding assays with functional assays involving phenotypic readouts: specifically pursuing compounds that bind and modulate various B-cell

master regulators including c-Myc and Pax5.

Angela Koehler, the Principle Investigator, is an Intramural Faculty member at the Koch Institute for Integrative Cancer Research, an associate member of the Broad Institute of MIT and Harvard, and a faculty co-advisor for the High Throughput Screening Facility at the Swanson Biotechnology Center. As MURJ found out in her interview, she is much more than a long list of titles. At MIT, she is a biological engineering professor and a strong leader in her field and has a deep passion for the academic and professional development of her students.

Dr. Koehler started her journey in STEM with a BA degree in Biochemistry and Molecular Biology from Reed College in 1997. There, she worked with structural and biochemical studies of proteins that recognize tRNA or DNA. In 2003, she received her PhD from Harvard University where she worked to develop novel technologies for identifying and characterizing interactions between proteins and small molecules.

The interview began with a bit more about her past and her focus for the future.

***MURJ: Thank you for meeting with us, Dr. Koehler. What do you think is one of the most important aspects of teaching undergraduate students?***

Dr. Koehler: I think that in order to keep students engaged, you need to entertain them. You would then care about and invest the time to learn about the subject material. If we just list equations, then people won't be interested. If there is no context, then students won't be inspired to think about the applications of their class material. The best way is to mix foundational knowledge students need to understand how mechanisms work with what can you do outside of the classroom. The material should give students the power to think about some kind of question – and allow them to question how they would go after it.

I actually want to teach more about the methods to modulate systems, and not so much about the mathematics underlying them. My background at Harvard was actually teaching biology majors the more chemically-oriented material.

I think one thing you worry about when teaching a course is striking

the balance between breadth and depth. Students need both. I make an effort to explain the overview of each module to relate cutting-edge literature to textbook material.

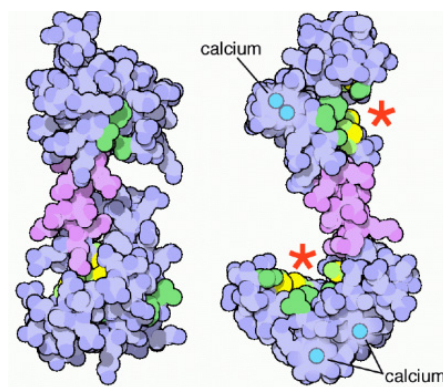
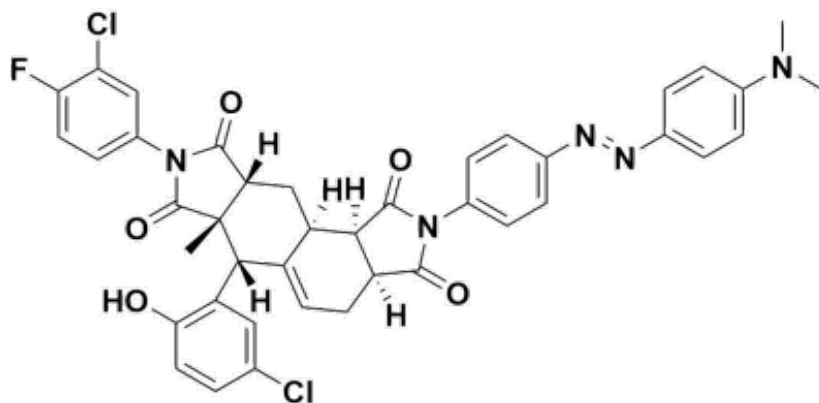
an impact in the life of a patient through basic science. Over time, I gravitated more and more towards chemistry – but always applied chemistry, thinking about how we can apply sciences to therapeutics.

*"Material should give students the power to think about some kind of question – and allow them to question how they would go after it."*

***MURJ: What was your path towards the career you have today?***

As an undergraduate at Reed College, I was originally in the biology department and thinking about a path towards becoming a physician. After some time, I realized after the first year that the parts of biology I liked the most were molecular in nature. I started to move a bit more towards Chemistry, but I actually hated chemistry at first. It was my least favorite first year class, but by the time I was a sophomore, I realized through conversations with a couple of people, one of whom was Richard Lerner, president of Scripps Research Institute in California that you could make

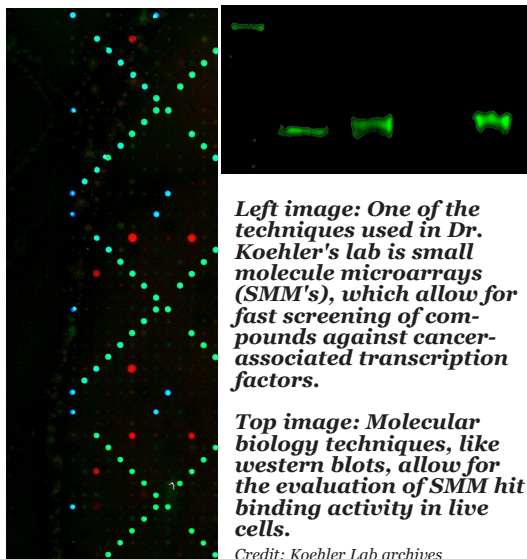
My thesis was about how these important transcription factors bind DNA. I became interested in dynamic systems: diseases are dynamic, development is a dynamic process. Through my undergraduate studies, I was learning about the compound, Colchicine in my organic synthesis class, cell biology and physiology. We were talking about how this was used as a tool to understand cell biology processes and how it was used in physiological studies, and how you could actually make it in my advanced organic class. I started to think that you can use these compounds to actually understand the dynamics of systems. But the problem is that for transcription factors there aren't a lot of ways to



***Dr. Koehler's lab discovers and develops direct small-molecule probes, such as calmoduphilin (left), for proteins involved in transcriptional regulation, including calmodulin (right).***

***Calmodulin is a calcium-binding protein which is essential in the regulation of many cellular processes, including inflammation, metabolism, and apoptosis.***

Credit: Koehler Lab archives



**Left image:** One of the techniques used in Dr. Koehler's lab is small molecule microarrays (SMM's), which allow for fast screening of compounds against cancer-associated transcription factors.

**Top image:** Molecular biology techniques, like western blots, allow for the evaluation of SMM hit binding activity in live cells.

Credit: Koehler Lab archives

study these mechanisms. So I went to Caltech in the lab of Barbara Imperiali, who is now a professor at MIT. I was there for a year and then I moved to Harvard Chemistry where I was enabled to build a technology that could be used for such "undruggable" targets. After leaving Harvard for my PhD, I became a Broad Institute Fellow where I started my first independent lab and we started to refine this technology. Today our group is trying to find small molecules that perturb oncogenic transcription factors. Can we use compounds to study these transcriptional factors that go awry in cancer and can we use compounds to clarify the relevance of these transcription factors in developmental and structural biology? So I discovered this interest in transcription factors as an undergrad and I am still studying them today. I actually tell my undergrads that as a Junior, when I was their age, I developed an interest, a question that seriously impacted the rest of my life. I never thought it would happen that way.

**MURJ:** So now that you are here at MIT, what do you like most about teaching and mentoring students?

I think it is great that literally every student I meet is not going

to class just to check it off a list, or using this experience at MIT as just a stepping-stone. People ask questions because they really care about them. They want to tackle the problem and really get to the root of it. I think that this genuine interest in trying to digest material because they want to use it to address problems they care about is so special at MIT. As a teacher, I want to arm students with the information and the thinking that will let them apply their learning so that they are posed to address the

upcoming problems in the world. MIT students really get that. I always challenge students to think about what is the main problem you see arising in the next 10, 20 years, and I urge them to go ahead and try to answer that question. Success is measured by impact, not simply the number of publications and patents that you have. This is not the case at every other institution so I love that.

**MURJ:** What about working with other professors?

I have been at other institutions where two professors in the same department are tackling the same problem and people become secretive and competitive. Their students don't interact. I think the philosophy here is that we are here to engage people with different expertise. You may need a physician scientist, chemist, and every single project in our lab at some point becomes a collaboration with

faculty members here at MIT and other hospitals around town. On this floor, we have several biologists and engineers and we have projects that connect to several groups here. We have equipment that connects the different labs too. I never thought that I would care about drug delivery and now we have a couple of projects in that field, and that is what is so unique to the Koch. We definitely love to collaborate on new projects here.

**MURJ:** Is your lab very diverse?

I appreciate not only diversity in terms of backgrounds, but also geographical and cultural diversity. We have had biologists, engineers, computer scientists and physicists in the lab and this is what actually makes us approach problems with a different perspective. Different people who have grown up in different parts of the world are also very important to the dynamic of our lab. We have also had people from Africa, Europe, South America, Asia, but actually no one from Australia...It is critical for the culture of our lab. So diversity is key not just in terms of degree, but also where they come from. Also we love age diversity. We have people in the lab who are older than I am but then we also have some high school students. It goes to prove that there are no stupid questions, and we want to foster that mentorship between more experienced researchers and students who are just starting out. By the way, the best time at our lab is during world cup soccer.

*"I think that this genuine interest in trying to digest material because [students] want to use it to address problems they care about is so special at MIT."*

Everyone has a lot of fun with the competition there.

**MURJ: Can you speak a little bit about who has been a really influential person in your life?**

This is actually so funny, because she is now here at MIT, but I would say Barbara Imperiali. I remember at CalTech having a conversation with her, and it really inspired me. If you really care about a problem, you should be fearless about trying any method. You will need to have others around you, but that if you really care, nothing should stop you. Looking back on that, that seems really smart and it has had a great impact on my career. And I tell this to all my students, 20 years later. So it is really nice to be able to be here again with her, and adopt this philosophy at MIT.

**MURJ: Where do you think the future of Biological Engineering is going?**

There are many many directions. The context that we talk about is human health, whether it is understanding how to rewire cells, come up with computational strategies to understand combinatorial effects of drugs, or better designing precision medicine. But there are other things too. There are opportunities to have a critical impact on agriculture. As climate shifts, we have new

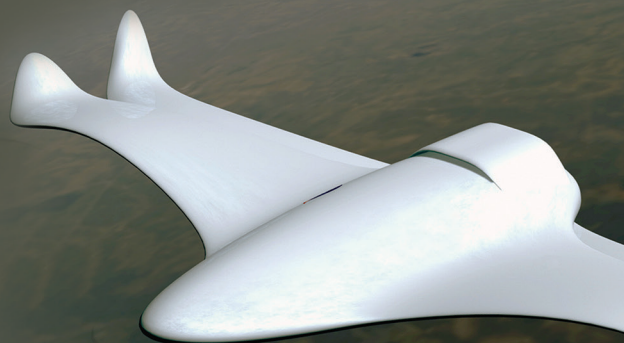
challenges in agriculture and energy needs. A lot of people are thinking about how can we take advantage of a framework of a biological system to impact energy production. I think there are many big problems. We should look for these big questions to apply the disciplines and the tools that will tackle these issues. It shouldn't be that we make tools and then find uses for them. And I think MIT is really focused on this initiative.

**MURJ: How has managing life and work been?**

Well, I have three kids and trust me, once you are managing three kids, everything else seems easy. I am really lucky because both my husband and I are researchers and chemists, and so we really get to work well as a team and juggle the little ones. But yeah, I changed three poop diapers before 7 AM this morning, so the rest of the morning is going to be great. It really helps you focus on your work with the time you have, and it makes you also appreciate your job, because you see how supportive the community can be. There was honestly some fear in my mind about how it would be perceived if I had a kid, but now I have three kids and everyone has been super helpful with every step of the way. ■



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# MURJ Reports

# *Impact of Neutron Resonance Elastic Scattering Energy Intervals on Nuclear Reactor Reactivity Calculations*

**Vivian Y. Tran<sup>1</sup>, Jonathan A. Walsh<sup>2</sup>, Prof. Benoit Forget<sup>3</sup>, Prof. Kord Smith<sup>4</sup>**

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**This study explores the impact of resonance elastic scattering on nuclear reactivity calculations through various treatments of the phenomenon in the OpenMC particle transport code. The results come from fresh fuel pin cell benchmark simulations, based on a BEAVRS-verified model of an operating light water reactor. The k-eigenvalues calculated from DBRC and ARES, two different but accurate treatments of resonant nuclides, are shown to be in excellent agreement (within 2 standard deviations). By applying the corrections only to the necessary energy intervals, a significant improvement in runtime can be achieved. In this work, those energy intervals are determined for the individual resonant nuclides present in the beginning of core, hot zero power pin cell.**

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## INTRODUCTION

The scattering cross sections of resonant nuclides can vary drastically within small energy intervals. In reactor physics simulations, accurate treatment of neutron resonance elastic scattering is vital, as the phenomenon can affect macroscopic values, such as the fuel temperature reactivity coefficients. Current methods that produce exact scattering kernels are computationally costly. It is the goal of this work to determine over what energy intervals it is necessary to apply the more accurate models of elastic scattering from resonant nuclides to improve computational efficiency without a loss of accuracy in results.

### OpenMC Particle Transport Code

OpenMC (Romano and Forget, 2013) is an open-source Monte Carlo neutron transport code that has been under active development at the Massachusetts Institute of Technology by the Computational Reactor Physics Group since early 2011. This code allows users

to build models and run simulations of nuclear reactor cores and other nuclear systems.

OpenMC has been shown to have excellent accuracy and scalability in criticality benchmark and full core eigenvalue calculations. OpenMC has been validated against several benchmarks in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) (NEA Nuclear Science Committee, 2009), as well as the full core Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS) (Horelik et al., 2013). Results obtained from OpenMC simulations have also been shown to agree well with those obtained from MCNP (X-5 Monte Carlo Team, 2009). OpenMC is available on GitHub (Romano, 2015).

### Resonance Scattering Phenomenon and Treatments

Correct treatment of the resonance elastic scattering is essential to the accuracy of reactor physics simulations. The differences of various methods for treating this

phenomenon can have significant effects on macroscopic values such as fuel temperature reactivity coefficients.

When modeling neutron-nuclide interactions, Monte Carlo neutron transport codes often make many assumptions. One such assumption relevant to resonance elastic scattering events that the reactor physics community has commonly made is that the  $K$  elastic scattering cross section of the nuclide is slowly varying at lower energies when determining the effect of temperature on the elastic scattering kernel. This assumption is a poor representation of nuclides with large scattering resonances. One verified way of correcting this assumption is the Doppler broadening rejection correction (DBRC) method (Rothenstein, 1996), which has been implemented in OpenMC. However, this method is computationally costly. A more efficient recently developed method, the accelerated resonance elastic scattering kernel (ARES) sampling method (Walsh, et al, 2014), has also been implemented in OpenMC and shown to agree well with the Doppler broadening rejection correction method. Since both methods appreciably slow down the code, the models' efficiency can be improved if the corrections are applied only when necessary for a particular class of reactors. This work looks at determining the energy ranges over which to apply the corrections, minimizing computation time, while still obtaining accurate eigenvalue results (which ensure that the integral effect of the resonance scattering phenomenon is captured satisfactorily).

In this work, we consider three methods for treating the resonance elastic scattering of neutrons: the constant cross section (CXS) model, the Doppler broadening rejection correction method, and the accelerated resonance elastic scattering kernel sampling method.

### Constant Cross Section Approximation (CXS)

Typically, stochastic treatment of resonance scattering assumes a constant cross section, independent of nuclide energy. However, this constant cross section model is largely inaccurate for heavy resonant nuclides, which can exhibit rapid cross section variation over small energy intervals.

### Doppler Broadening Rejection Correction (DBRC)

To correct for this approximation, a Doppler broadening rejection correction method was developed (Rothenstein, 1996). This method samples a Maxwellian target velocity distribution and then performs rejection sampling on a  $0\text{ K}$  scattering cross section, which can be extremely inefficient in the vicinity of resonances. DBRC has previously been shown to accurately treat the resonance scattering.

### Accelerated Resonance Elastic Scattering (ARES)

An alternate treatment with improved efficiency has also been implemented in OpenMC. Unlike DBRC, this method directly samples the  $0\text{ K}$  scattering cross section distribution and then performs a rejection sampling of a Maxwellian distribution. The ARES method minimizes the number of rejected values and consequently reduces the required computation time.

This work will provide further validation of the ARES method against the DBRC method in their treatments of resonance scattering for individual nuclides. However, both are still significantly more computationally costly than the CXS model. Therefore, it is advantageous to apply the corrections only when necessary and default to the CXS approximation when appropriate. If the energy ranges over which to apply the corrections are minimized for each of the nuclides present in the system, computation time can be significantly reduced.

## RESULTS

First, this paper serves to demonstrate that the ARES method does in fact correctly reproduce exact scattering kernels, as the DBRC method does. Next, we show how the correct treatment of the resonance scattering phenomenon affects both integral quantities such as the effective multiplication factor, and differential quantities such as average post-collision energy and upscatter probability. The results of this study demonstrate that the two methods produce agreeing values for  $k_{\text{eff}}$  within acceptable statistical uncertainties at the  $\sim 10\text{ pcm}$  level. Furthermore, with the goal of minimizing computation time, the energy ranges over which the corrections should be applied are determined individually for each nuclide with multiple resonances below  $1000\text{ eV}$ .



**Figure 1.** Plotted from OpenMC, a 2D, infinite lattice pin cell modeled with reflective boundary conditions.

## Model Details

The simulations discussed in this paper are based on the BEAVRS model of a real, operating pressurized water reactor. For the purposes of this study, it is not necessary to simulate the whole system, thus a single pin will be used.

The pin cells modeled in these simulations are beginning-of-core (BOC) hot-zero-power (HZIP) pin cells, as shown in Fig. 1. These fresh fuel pin cells have been modeled with reflective boundary conditions. The full core model is that of the BEAVRS reactor.

Since the system modeled is a light water reactor (LWR), the results of these tests can be generalized to other LWRs, which make up an overwhelming majority of operating commercial power reactors in the United States.

## Comparison of Methods: Scattering Kernels, Average Energies, Upscattering Probabilities

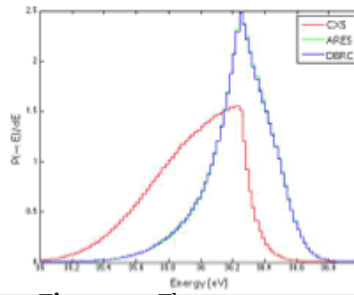
In Figs. 2 & 3, scattering kernels for two s-wave resonances of U-238 are plotted from results using the three different methods.

From these plots, it is clearly evident that the CXS approximation is a very poor model of the cross section near resonant energies. However, the DBRC and ARES methods correctly treat the resonances and very closely converge with one another. The correct treatment of these resonance elastic scattering cross sections is vital to the reactivity calculation of the system, as they have a strong affect on resonance absorption rates.

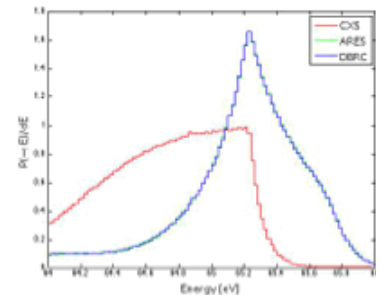
The differences in these three treatments also affect other important values, such as the average neutron energy after scattering and the probability of upscattering. Comparisons of the average energy after scattering for each of the three different methods for incident energies near selected U-238 resonances are listed in Table I.

While the average energies after scattering calculated from each of the three methods mostly agree, there is a much closer agreement between ARES and DBRC than CXS. Since DBRC has been verified to accurately treat the resonance elastic scattering phenomenon in Monte Carlo codes, it is worthwhile to note that results from ARES more closely agree with those obtained from DBRC than the CXS-calculated values do.

Similar comparisons of the upscattering probabilities at resonances for each of the three different methods for eight prominent resonances of U-238 are listed in Table II.



**Figure 2.** The resonance scattering kernels for the 36.68 eV s-wave resonance of U-238 for neutrons at incident energies of 36.25 eV are plotted from the CXS approximation, DBRC method, and ARES method.



**Figure 3.** The resonance scattering kernels for the 66.13 eV U-238 s-wave resonance for incident neutrons at 65.23 eV are plotted using CXS, ARES, and DBRC.

While the DBRC and ARES probabilities agree very closely, the probabilities obtained from the CXS approximation are grossly inaccurate. Because the constant cross section approximation is inaccurate for heavy resonant nuclides such as U-238.

These results, especially the differences in upscattering probabilities and generation of scattering kernels, further demonstrate that the CXS approximation is a poor choice for treating the resonance elastic scattering phenomenon and illustrates how this method could impact important system characteristics. Simultaneously, results also further validate the ARES method against the DBRC method in its accurate treatment of resonance elastic scattering.

Average Energy After Scattering (eV)			
Incident Energy (eV)	CXS	DBRC	ARES
6.52	6.48	6.61	6.61
20.2	20.04	20.03	20.04
36.25	35.96	36.25	36.25
65.23	64.76	65.22	65.22
100.8	100.23	100.38	100.39
186.6	186.1	186.12	186.12
207.6	207.1	207.13	207.13
236.5	236.05	236.07	236.07

**Table I.** Average energy after scattering in the vicinity of resonances for U-238.

## Applying Corrections: Energy Ranges Based on Eigenvalue Calculations

Applying the DBRC and ARES corrections to all resonant nuclides present in the system will lead to more practical and realistic results. However, since both corrections are computationally costly, it is advantageous to apply the corrections to the minimum energy range

<i>Upscattering Probabilities (%)</i>			
Incident Energy (eV)	CXS	DBRC	ARES
6.52	29.4	84.42	84.42
20.2	13.31	22.93	23.26
36.25	10.26	40.01	40.48
65.23	6.59	50.51	50.66
100.8	4.6	10.69	10.83
186.6	6.54	8.28	8.38
207.6	5.08	8.67	8.65

**Table II.** The probability of neutron upscattering near s-wave resonance energies for U-238.

necessary to still achieve accurate results. These energy ranges can vary significantly from nuclide to nuclide and result in different costs in computation time. Therefore, it is best to determine what energy ranges to apply the corrections for each nuclide individually.

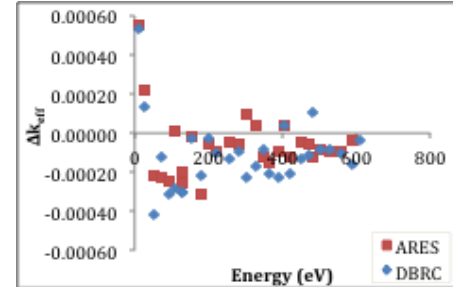
The simulations conducted for this work are done individually for each nuclide to determine the optimal energy range. For each simulation, 1,000,000 particles were simulated per batch, 25 inactive batches were discarded, and results were tallied for the subsequent 100 active batches.

The process by which the energy range is determined is based on an effective multiplication factor reference case achieved from applying the corrections from 0.01 – 1000 eV. Below 0.01 eV and above 1000 eV, the CXS approximation is applied. To ensure optimal accuracy in the reference case, 10,000,000 particles per batch were simulated, ten times more than our standard simulations. The upper bound of these base cases is chosen to be 1000 eV, because results showed that there were minimal differences in  $k_{\text{eff}}$  when the upper bound was increased.

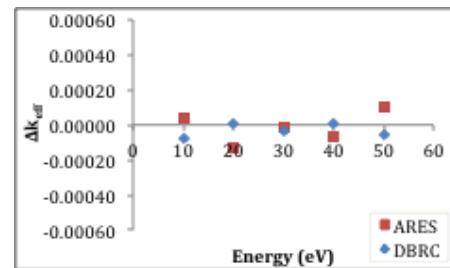
To find the optimal energy range over which to reduce the application of the corrections, the energy range begins at a minimum energy of 0.01 eV, and the upper energy is set such that it fully encloses the first s-wave resonance of the nuclide, then the second, and so on. The upper energy of these ranges is determined by calculating the median values between two consecutive resonance energies. The resonance energies were obtained online from the National Nuclear Data Center (Herman, 2015). For nuclides without resonances below 1000 eV, such as Cr-50, Sn-120, Sn-122, and Sn-124, the constant cross section model will serve as an accurate approximation.

The upper bounding energy is continually increased to enclose the next resonance until the resulting  $k_{\text{eff}}$  is shown to agree to within 2 of the reference result. For nuclides

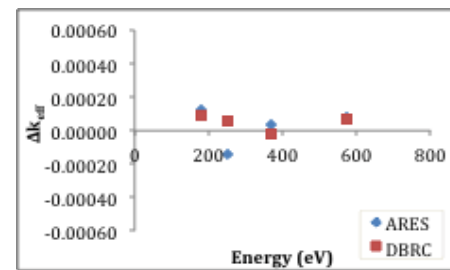
with resonances very close together, such as U-235,  $E_{\text{max}}$  was increased at a step interval of 10 eV for each succeeding simulation. To prevent any false convergence in these values, the  $E_{\text{max}}$  is determined to be the second consecutive energy in which the resulting  $k_{\text{eff}}$  is within



**Figure 4.** Differences in  $k_{\text{eff}}$  at various energies compared to the  $k_{\text{eff}}$  calculated from the reference case (from 0.01 – 1000 eV, with 107 particles per batch) are plotted for U-238. One can see that the energies fall within statistical deviations at around 200 eV.



**Figure 5.** Differences in  $k_{\text{eff}}$  at various energies compared to the  $k_{\text{eff}}$  calculated from the reference case (from 0.01 – 1000 eV, with 107 particles per batch) are plotted for U-235. The  $k_{\text{eff}}$  values converge to the reference case at around 20 eV.



**Figure 6.** Differences in  $k_{\text{eff}}$  at various energies compared to the  $k_{\text{eff}}$  calculated from the reference case (from 0.01 – 1000 eV, with 107 particles per batch) are plotted for Sn-119. The  $k_{\text{eff}}$  values converge within two standard deviations at around 250 eV.

tight statistical uncertainties. The difference between these two values for each successive resonance is plotted for U-238 in Fig. 4, for U-235 in Fig. 5, and for Sn-119 in Fig.

6. Evidently, the energy ranges over which it is necessary to apply the DBRC and ARES corrections for these nuclides vary significantly. If the energies were not individually determined, applying a general range could greatly decrease computational efficiency.

In Table III, each resonant nuclide present in the beginning-of-core (BOC) system is listed along with its determined  $E_{\max}$ , the difference in  $k_{\text{eff}}$  from the reference case, and the associated standard deviation for both the DBRC and ARES methods.

The results in Table III demonstrate the variability of the necessary energy ranges over which to apply the corrections for different nuclides. For all nuclides, DBRC and ARES agree on the upper bound of the energy.

Comparisons of results obtained from DBRC and ARES show they are in excellent agreement to within 1-2.

### Verification of Determined Energy Ranges

Shifting our investigation from individual nuclides in the pin cell to all nuclides present in the BOC-HZP pin cell, the computational efficiency of minimizing the energy ranges becomes significantly noticeable.

Table IV lists results from simulations using the CXS approximation and applying the DBRC and ARES

Nuclide	Method	$E_{\max}$	$\Delta k_{\text{eff}}$	$1\sigma$
Zr-91*	DBRC	486.92	0.00000	0.00010
	ARES	486.92	0.00007	0.00009
Sn-112	DBRC	79.73	-0.00012	0.00008
	ARES	79.73	0.00015	0.00008
Sn-114	DBRC	825	0.00002	0.00010
	ARES	825	-0.00005	0.00009
Sn-115	DBRC	370.4	0.00009	0.00010
	ARES	370.4	0.00009	0.00010
Sn-116*	DBRC	1000	0.00011	0.00009
	ARES	1000	-0.00008	0.00009
Sn-117	DBRC	122.22	-0.00004	0.00010
	ARES	122.22	-0.00008	0.00010
Sn-118*	DBRC	1000	-0.00003	0.00009
	ARES	1000	0.00000	0.00009
Sn-119	DBRC	252.795	0.00006	0.00010
	ARES	252.795	-0.00014	0.00009
U-234	DBRC	23.08	-0.00005	0.00009
	ARES	23.08	-0.00005	0.00009
U-235**	DBRC	20	-0.00008	0.00010
	ARES	20	0.00007	0.00008
U-238	DBRC	255.53895	-0.00002	0.00009
	ARES	255.53895	-0.00009	0.00008

Table III. Energy ranges to apply DBRC and ARES corrections for each resonant nuclide.

\*These nuclides only had one resonance below 1000 eV.

\*\*The resonance energies of these nuclides were very close together, so a step size of 10 eV was taken in an effort to minimize the energy range.

Method	$E_{\max}$ (eV)	$k_{\text{eff}}$	$1\sigma$
CXS	1000	1.35601	.00009
**	1000	1.35536	.00010
ARES	1000	1.35537	.00009
DBRC	--*	1.35536	.00010
ARES	--*	1.35537	.00008

Table IV.  $k_{\text{eff}}$  values from simulating all resonant nuclides in the BOC-HZP pin cell.

\* $E_{\max}$  for each nuclide taken from the determined  $E_{\max}$  listed in Table III.

corrections over the comparison energy range of 0.01 – 1000 eV, and results from applying the corrections over the determined optimal upper energy bounds for each nuclide, as listed in Table III.

The calculated  $k_{\text{eff}}$  value using the CXS approximation is significantly higher than the  $k_{\text{eff}}$  values obtained from treating the neutron resonance elastic scattering phenomenon correctly. When applying the DBRC and ARES corrections only from 0.01 eV to the determined upper bounds as listed in Table III, the results are exactly the same as those obtained from applying the corrections over a larger range from 0.01 to 1000 eV. The differences in the calculated  $k_{\text{eff}}$  values from using the DBRC and ARES corrections are also well below 1.

### Conclusion

This study explores the impact of resonance elastic scattering on nuclear reactivity calculations through various treatments of the phenomenon in the OpenMC particle transport code. The results come from fresh fuel pin cell benchmark simulations, based on the BEAVRS model of an operating light water reactor. The k-eigenvalues calculated from DBRC and ARES, two different but accurate treatments of resonant nuclides, are shown to be in excellent agreement (within 2 standard deviations). By applying the corrections only to the necessary energy intervals, a significant improvement in runtime can be achieved. In this work, those energy intervals were determined for the individual resonant nuclides present in the beginning of core, hot zero power pin cell. Applying the corrections over these determined energy intervals to light water reactor simulations treating all resonant nuclides in the system reduced computation time, while resulting in no loss of accuracy. Future work may include looking at systems with different nuclides and quantifying the overhead runtime that is saved by a limited application of the exact treatments. A closer investigation into comparing the reaction rates of the various nuclides could provide a more detailed measure of the impact of applying exact resonance scattering treatments over extended ranges.

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# *Creation of a Model to Predict Plant Hydrocyclone Performance Using Computational Fluid Dynamics*

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**This report highlights the creation of a simulation model in ANSYS FLUENT™ to predict the separation performance of a plant hydrocyclone. The complex three-phase flow within the hydrocyclone was carefully addressed using various methodologies. The internal flow field was initialized using the Reynolds stress turbulence model and the air core was generated using the Volume of Fluid multiphase model; particle interactions with the continuous phase were resolved using the Eulerian-Lagrangian particle tracking method and one-way coupling. The flow split and particle collection efficiency were then compared to existing industrial data; the simulation results showed reasonable agreement with the experimental data, but additional work must be done to determine whether the deviation from the experimental data is due to model inadequacies or geometric factors.**

## 1. Introduction

Hydrocyclones are one of the most commonly used classifying devices for materials separation. They have been commonly used in industry since the 1940's with the first US Patent for a hydrocyclone dating back to 1891 (Bretnai, 1891). Today they are used in a variety of applications such as mineral processing, where they are used to differentiate between gangue and valuable metals, and the oil industry, where they are used to separate oil from water and particulates. Hydrocyclones can be separated into two main categories, classifying cyclones and dense medium cyclones. Classifying cyclones differentiate particles based on their size whereas dense medium cyclones separate particles primarily based upon their density. Both types of cyclones operate based on the same fundamental principles.

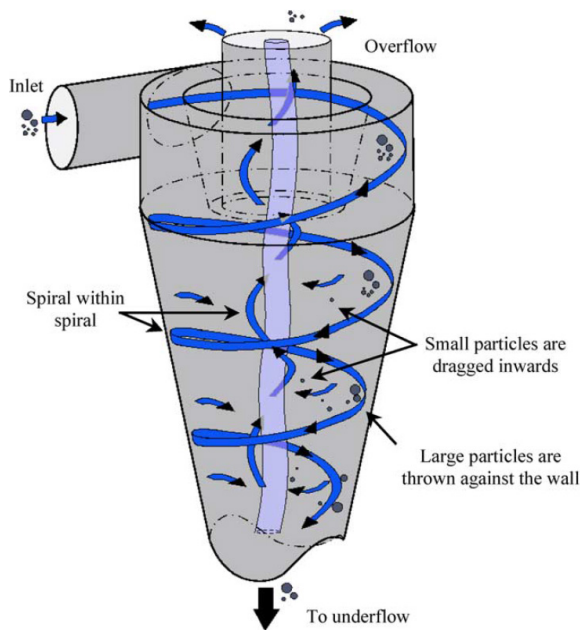
Slurry is fed into the hydrocyclone via one or more tangential inlets which creates a forced vortex within the cyclone body. Due to the decrease in volume in the conical section of the cyclone, the flow in this region reverses and creates a secondary inner vortex. The strong centrifugal forces generated by the swirling fluid result

in a radial distribution of pressure that is low in the center of the cyclone and high near the walls. When the pressure drops below ambient atmospheric pressure, air is sucked into the cyclone via the underflow resulting in the generation of a central air core.

Particles trapped in the circulating flow are subjected to both gravitational and centrifugal forces; the centrifugal forces dominate during classification and can be on the order of 500g. (Brennan, 2009) Larger/ denser particles migrate towards the outer walls and smaller/less dense particles migrate towards the inner core. As a result, larger particles tend to be discharged via the underflow while smaller particles are discharged via the overflow. (Aldrich, 2015) See (Figure 1)

## 2. Grid Generation

The geometry of the simulated hydrocyclone was specified by a small diameter commercial classifying hydrocyclone; however, for confidentiality reasons the dimensions must be omitted. The geometry resembles classic cyclone theory with a single circular tangential inlet, a cylindrical body leading into a conical section,



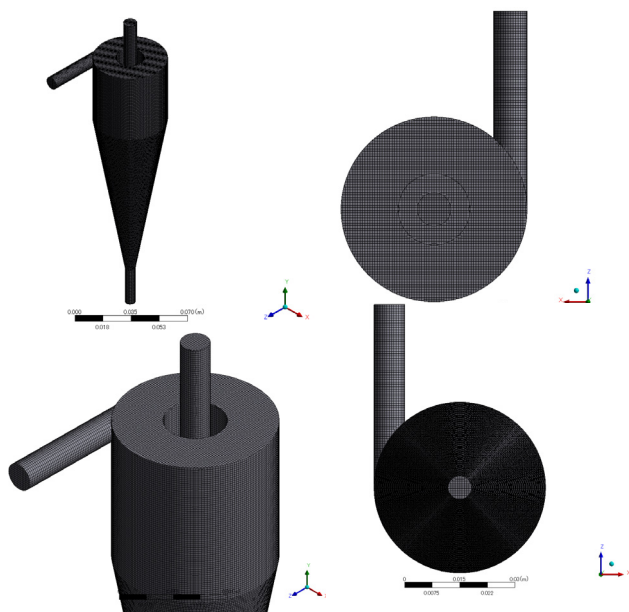
**Figure 1.** The figure above shows the fundamental operation of a hydrocyclone. Water enters from the tangential inlet at the top and is forced into a vortex by the curvature of the cyclone body. At the bottom of the cyclone, the flow reverses and a secondary vortex forms. Due to the formation of low pressure zone at the center of the cyclone, air is sucked into the system and forms an air core. Particle separation occurs due to centrifugal forces with large particles being discharged through the underflow and small particles being discharged through the overflow. Figure credit: (Cullivan, 2004)

and a vortex finder that protrudes into the body. Because this geometry resembles cyclone theory it was expected to utilize the same separation mechanisms as normal classifying hydrocyclones and was modeled as such.

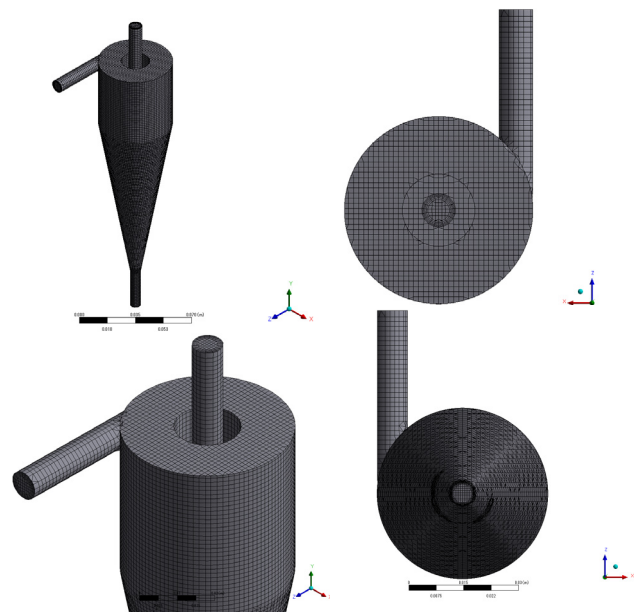
Two different computational meshes were created for these simulations: a rougher mesh consisting of 153,225 elements and a finer mesh consisting of 584,706 elements. Both meshes were unstructured hex and were generated utilizing the CutCell algorithm in ANSYS Meshing. (Slack, 2004) reported that a tetrahedral mesh is too diffusive for highly convective flows; this false diffusion can lead to large deviations in the simulated results. Thus it is the best practice to align the mesh with the flow direction and this task can only be accomplished with hex elements. CutCell algorithms generate excellent quality uniform hex meshes throughout most of the domain, but they struggle to capture details near the boundaries. Due to this shortcoming, extra care was taken to refine the mesh near the cyclone walls.

As evident in (Figure 2), the cell sizes in the refined mesh were almost perfectly uniform in size throughout the computational domain. It was particularly important to have uniform mesh because (Seo, 2014) stated that it is a requirement for the VOF model. The fine mesh had significantly more elements than most previous hydrocyclone simulations, (Table 1), thus the results should more accurate.

A grid independency test revealed that the fine mesh and rough mesh yielded the same final flow splits, but



**Figure 2.** This figure shows the fine computational mesh generated with the CutCell algorithm for these simulations. This unstructured hex mesh is uniform in size throughout the entire domain and accurately captures the geometry of the cyclone.



**Figure 3.** This figure shows the rough computational mesh generated with the CutCell algorithm for these simulations. This unstructured hex mesh is uniform in size throughout most of the domain but it needed inflation layers to accurately capture the boundary features.

Name	Year	Mesh Type	Structured	Number of Elements
Ghodrat	2014	Hex	Yes	195,268
Hwang	2013	Hex	No	150,000
Karimi	2012	Hex	Yes	226,724
Murthy	2012	Hex	No	150,000
Azadi	2010	Hex	Yes	160,000
Brennan	2009	Hex	Yes	1,330,000
Brennan	2006	Hex	Yes	2,510,000
Bhaskar	2006	T-Grid	No	150,000
Cullivan	2004	Hex	No	99,776

**Table 1.** This table shows the distribution of mesh sizes in recent CFD simulations of hydrocyclones.

Mesh	Type	Structured	Method	Inflation
Rough	Hex	No	CutCell	Yes 5 Layers
Fine	Hex	No	CutCell	No
Mesh	Body Sizing	Skewness MAX	Orthogonal Quality MIN	Cell Count
Rough	0.002m	0.93	0.056	153,225
Fine	0.001m	0.842	0.248	584,706

**Table 2.** This table shows the details of the simulated meshes. The rough mesh generated for these simulations has the same number of elements determined by past investigations to be grid independent and the fine mesh generated has far more elements than required to ensure accuracy of the simulations.

the fine mesh was chosen for the remaining simulations because its uniform mesh allowed the VOF model to converge much faster.

A summary of grid details can be found in (Table 2).

### 3. Model Description

#### 3.1 Turbulence Modeling

ANSYS FLUENT utilizes the Reynolds averaged Navier Stokes equations to model turbulence. During Reynolds averaging the flow variables of the incompressible Navier Stokes equations are separated into a time averaged and a fluctuating component. After substituting these components into the continuity and momentum equations and ensemble averaging, the equations take on the form in Equation 1. The Reynolds stresses  $\rho \overline{u'_i u'_j}$  need to be modeled in order to close the momentum equation.

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0$$

$$\rho \left[ \frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} \right] = - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \mu \frac{\partial \bar{u}_i}{\partial x_j} - \rho \overline{u'_i u'_j} \right)$$

#### Equation 1: RANS Continuity and Momentum

The Reynolds stress model is one of the most complex turbulence models for the RANS equations. Unlike the k-ε model, the Reynolds stress model does not assume isotropic turbulence and instead solves a transport equation for each Reynolds stress component. (Iaccarino, 2004) This method makes computations much more difficult; for three dimensional simulations, this model requires seven additional transport terms for the Reynolds stresses.

$$\frac{\partial}{\partial t} (\rho \overline{u'_i u'_j}) + \frac{\partial}{\partial x_k} (\rho u_k \overline{u'_i u'_j}) =$$

Local Time Derivative and Convection

$$- \frac{\partial}{\partial x_k} (\rho \overline{u'_i u'_j u'_k} + \overline{p' (\delta_{kj} u'_i + \delta_{ik} u'_j)})$$

#### 1. Turbulent Diffusion

$$+ \frac{\partial}{\partial x_k} \left[ \mu \frac{\partial}{\partial x_k} (\overline{u'_i u'_j}) \right]$$

#### 2. Molecular Diffusion

$$- \rho \left( \overline{u'_i u'_k} \frac{\partial \bar{u}_j}{\partial x_k} + \overline{u'_j u'_k} \frac{\partial \bar{u}_i}{\partial x_k} \right)$$

#### 3. Stress Production

$$- \rho \beta (g_i \overline{u'_j \theta} + g_j \overline{u'_i \theta})$$

#### 4. Buoyancy Production

$$+ \rho' \left[ \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right]$$

#### 5. Pressure Strain

$$-2\mu \frac{\partial u'_i}{\partial x_k} \frac{\partial u'_j}{\partial x_k}$$

### 6. Dissipation

$$-2\rho\Omega_k (\overline{u'_j u'_m} \varepsilon_{ikm} + \overline{u'_i u'_m} \varepsilon_{jkm})$$

### 7. Production from System Rotation

#### Equation 2: Reynolds Stress Model

(FLUENT Theory Guide, 2012)

### 3.2 Multiphase Modeling

The presence of an air core in the center of the cyclone chamber dictates the final flow distribution and particle separation efficiency. A multiphase model is necessary to capture this phenomenon. The Volume of Fluid Model has many benefits over the mixture model for this application. In particular, the VOF model only solves one set of momentum equations for the entire domain which eases the computational requirement. Additionally, the VOF model treats the two fluids as immiscible which leads to a clear air water interface. (FLUENT Theory Guide, 2012)

$$\begin{aligned} & \frac{\partial}{\partial t} (\rho \vec{v}) + \nabla * (\rho \vec{v} \vec{v}) \\ &= -\nabla p + \nabla * [\mu (\nabla \vec{v} + \nabla \vec{v}^T)] + \rho \vec{g} + \vec{F} \end{aligned}$$

#### Equation 3: VOF Momentum

(FLUENT Theory Guide, 2012)

The VOF model tracks the movement of air water interface with a volume fraction continuity equation. The equation takes the form of:

$$\frac{1}{p_q} \left[ \frac{\partial}{\partial t} (\alpha_q \rho_q) + \nabla * (\alpha_q \rho_q \vec{v}_q) \right] = S_{\alpha_q} + \sum_{p=1}^n (\dot{m}_{pq} - \dot{m}_{qp})$$

#### Equation 4: Volume Fraction Equation

(FLUENT Theory Guide, 2012)

$\dot{m}_{qp}$  and  $\dot{m}_{pq}$  represent the mass transfer from phase q to p and p to q. In this simulation air is represented by q and water by p. Only the volume fraction of the secondary phase is calculated with the primary phase volume fraction being equal to  $1 - v_{iq}$ . The momentum equation depends on the volume fraction of these phases because the phases have different densities and viscosities.

### 3.3 Discrete Phase Modeling

Particle motion through the cyclone body is described using the Euler-Lagrange approach to discrete phase modeling. In DPM, particles trajectories are calculated by integrating the following force balance equation written in the Lagrangian reference frame:

$$\frac{du_p}{dt} = F_D (\vec{u} - \vec{u}_p) + \frac{\vec{g}(\rho_p - \rho)}{\rho_p} + \vec{F}$$

In this equation F is the additional acceleration term and  $F_D$  is the drag force acting on each unit mass. This drag force can be expressed as:

$$F_D = \frac{18\mu C_D Re}{\rho_p d_p^2 * 24}$$

with Re, the relative Reynolds number, being defined as:

$$Re = \frac{\rho d_p |\vec{u}_p - \vec{u}|}{\mu}$$

#### Equation 5: Particle Force Balance

(FLUENT Theory Guide, 2012)

A one-way coupling scheme between the discrete and continuous phase was chosen because the injections were very dilute. In one-way coupling, the continuous phase influences the discrete phase via drag and turbulence but the discrete phase does not influence the continuous phase. This coupling scheme is computationally beneficial for dilute injections but two-way coupling must be used at higher volume fractions.

## 4. Simulation Parameters

The hydrocyclone simulations were conducted in three stages as follows: Flow Field Development, Air Core Generation, and Particle Injections. (Brennan, 2006) described the advantages of a multiple step approach but the procedure in this paper differs slightly from his.

In all of the following experiments, the SIMPLE discretization scheme was used for pressure velocity coupling, PRESTO was used for pressure, and QUICK was selected for everything else. The modified HRIC and the Compressive discretization schemes for volume fraction were compared and gave nearly identical results; however, since Modified HRIC was faster to compute it was utilized for all of the air core simulations. Bounded

Second Order Implicit was used as the transient formulation.

The tangential inlet was given a velocity inlet boundary condition and the overflow, as well as the underflow, was given a pressure outlet boundary condition with the radial pressure distribution option enabled. The water used in the simulations had the default density and viscosity defined by the FLUENT database (998.2 kg/m<sup>3</sup> and 1.003\*10<sup>-3</sup> kg/m-s respectively.)

#### 4.1 Flow Field Development

In the first stage, the cyclone was initialized with the entire domain filled with water and with no air present. The Reynolds Stress Model with the Linear Pressure Strain option enabled was selected as the turbulence model. The simulation ran for 2000 time steps at a step size of 1\*10<sup>-3</sup> s; at 2000 time steps a low pressure region had formed in the center of the cyclone and both the primary and secondary vortex were clearly visible.

#### 4.2 Air Core Generation

After the flow field was initialized, the VOF model was activated and the backflow air volume fraction of the overflow and underflow was set as 1. The simulation ran for another 20,000 time steps with a time step of 1\*10<sup>-4</sup> s. During this time, air entered through both outlets to create the air core. The flow split and pressure drop was observed to reach steady state after a total simulated time of 4s.

#### 4.3 Particle Injections

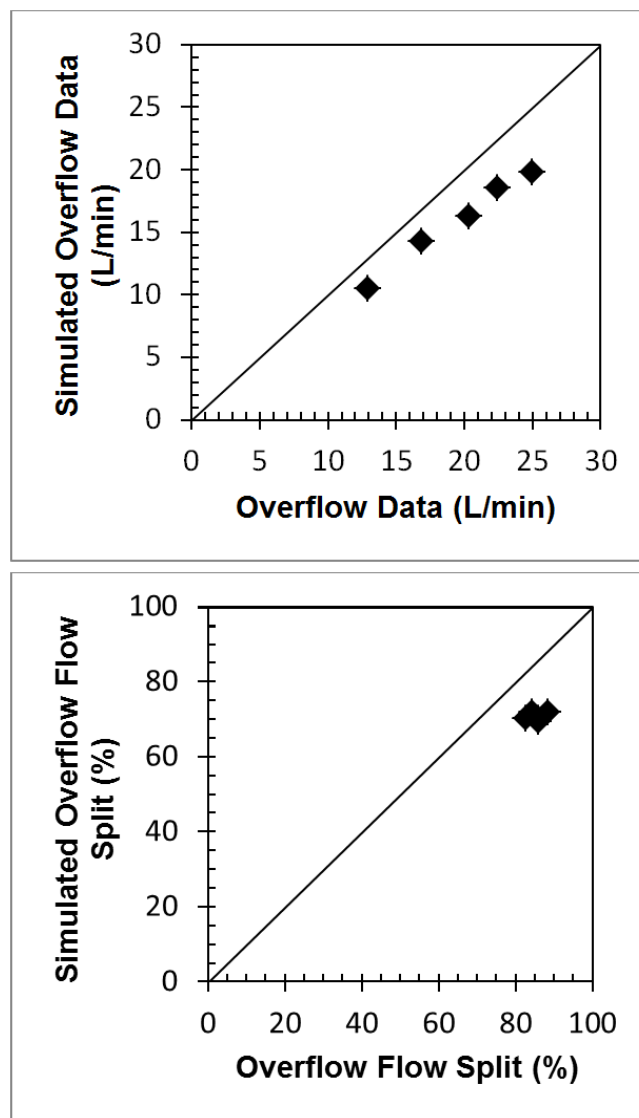
During the final stage, the DPM was enabled and particle injections began. The injections were defined as a surface injection from the velocity inlet and the particles were allowed to interact with the continuous phase. (Cullivan, 2004) highlighted the importance of the integral length scale on particle tracks; he reported that an integral length of 1\*10<sup>-5</sup> m was sufficient to ensure that the statistical destination of the particles was independent of the length scale. Thus this integral length was enabled for these simulations.

### 5. Results and Discussion

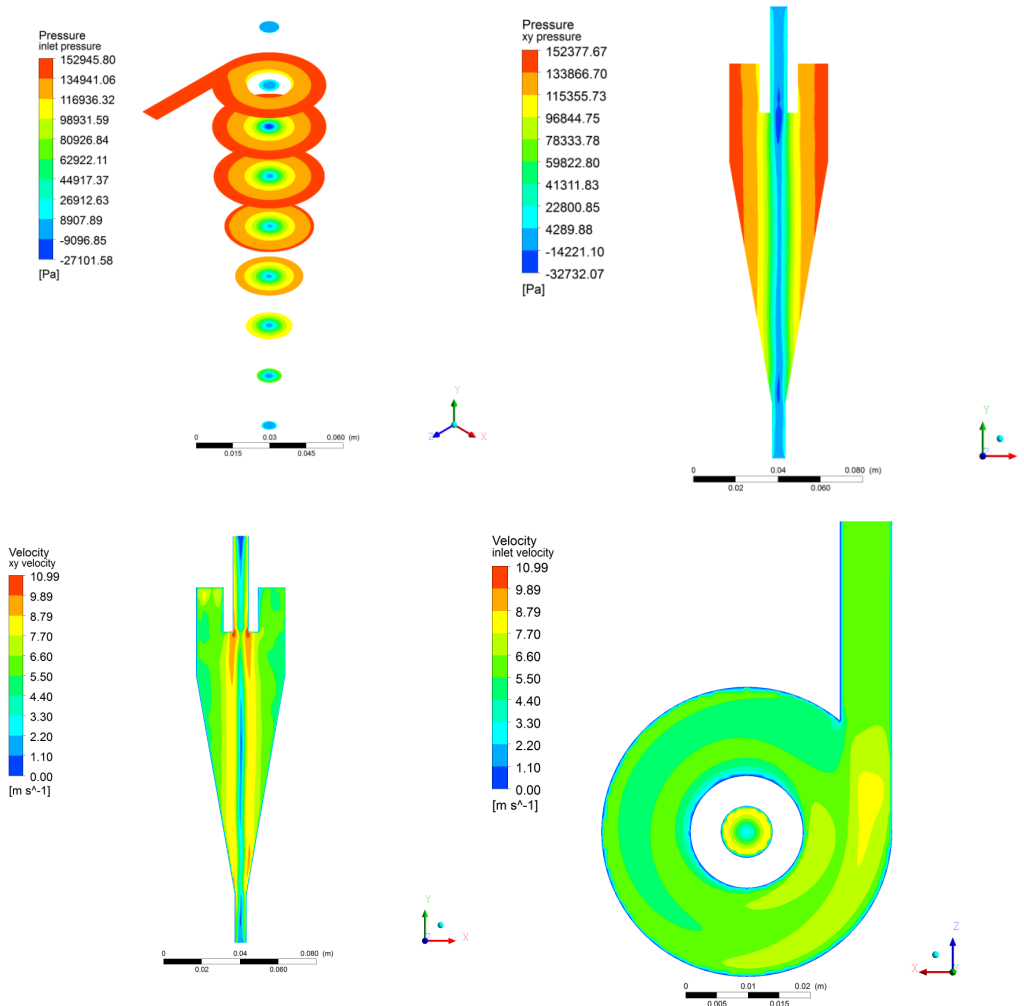
#### 5.1 Model Validation

It is necessary to compare the simulated results to experimental data to validate that the model is predicting the flow behavior correctly. Industrial data was provided for the commercial hydrocyclone operating without an

air core at 5 different flow rates: 15, 20, 23, 27, and 29 L/min. Data from the first stage of simulations was compared to the provided data and then plotted. As evident in (Figure 4), the simulation model clearly captures the trend reported by the industrial data but the flow split to the overflow is consistently under predicted. (Delgadillo, 2005) reported that in his simulations the RSM under predicted the flow split to the overflow by 10.6%. In these simulations the flow split to the overflow was under predicted by an average of 15.7±2.1% which is slightly larger than the deviation reported by (Delgadillo, 2005) but it is close enough that most of the deviation can be attributed to the choice of turbulence model.



**Figure 4.** This figure shows the results of a simulation benchmark. From the graphs above, it is evident that the trends generated by the simulated cyclone closely match the results from the physical cyclone; the matching trends validate the model for future simulations.



**Figure 5.** The figure at left shows the distribution of pressure once the primary flow stabilized. As anticipated, we can clearly observe a radial pressure gradient that is low in the center and high near the walls of the cyclone.

**Figure 6.** The figure at left shows the distribution of velocities in the cyclone body. A high velocity region exists near the vortex finder because secondary vortex is being compressed in order to flow through the overflow and because some water from the inlet prematurely exits through the overflow.

Commercial Data		Simulated Data		Deviation	
Inlet (L/s)	Overflow (L/s)	Inlet (L/s)	Overflow (L/s)	Inlet (L/s)	Overflow (L/s)
15	13	14.9	10.3	0.1	2.7
20	17	19.8	14.2	0.2	2.8
23	20.5	22.8	16.3	0.2	4.2
27	22.5	26.4	18.4	0.6	4.1
29	25	28.3	19.8	0.7	5.2

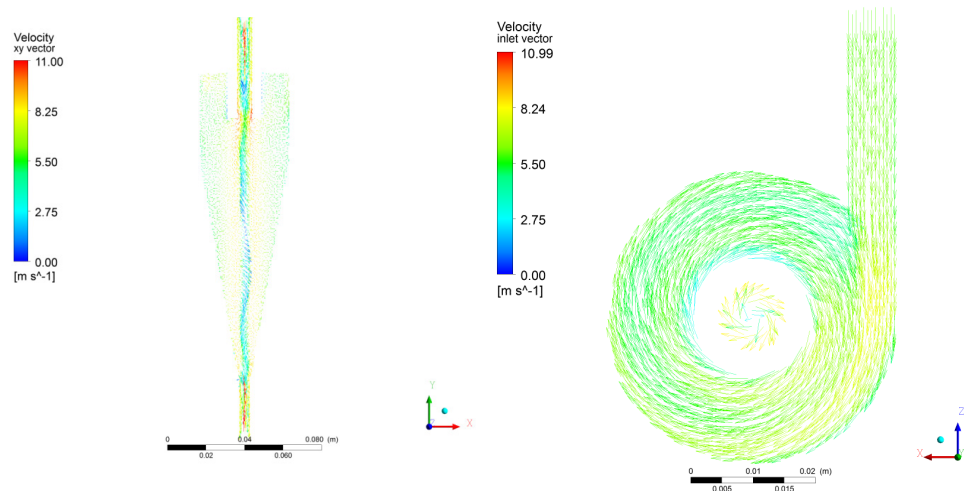
**Table 3.** This table details the volumetric flow split data generated from a benchmark where the simulated results are compared to commercial data.

It is important to note here that the additional deviation could have been caused by minute differences in geometry. The simulated cyclone was an operating cyclone which had inherent differences in geometry due to manufacturing tolerances and it likely experienced

Commercial Data		Simulated Data		Deviation
Inlet (L/s)	Overflow (%)	Inlet (L/s)	Overflow (%)	Overflow (%)
15	86.7	14.9	69.3	17.4
20	85	19.8	71.6	13.4
23	89.1	22.8	71.3	17.8
27	83.3	26.4	69.8	13.5
29	86.2	28.3	69.8	16.4

**Table 4.** This table details the volumetric flow split data generated from a benchmark where the simulated results are compared to commercial data.

erosion during use. This coupled with the difficulty of measuring dimensions of cyclones in situ could account for the additional deviation, but a second investigation using LES discretization is necessary to see if the additional deviation is constant.



**Figure 8.** This figure shows the axial and radial velocity vectors in the cyclone body. From these images, it is obvious that the cyclone geometry creates a strongly swirling flow and that the flow reverses in the middle of the conical section.

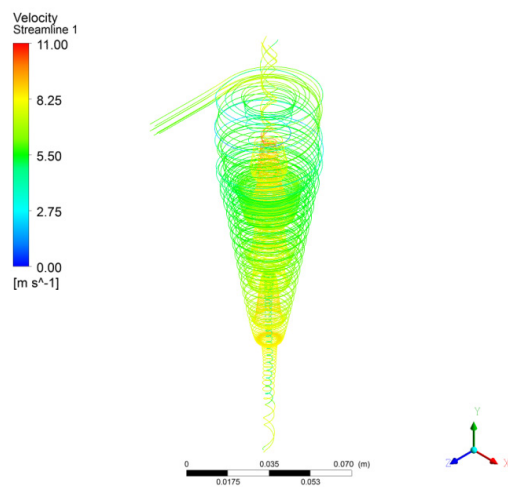
If we examine the axial contours of static pressure and the velocity at this stage, we can see that the flow behavior follows our expectations for cyclones. In (Figure 5), a well-defined pressure gradient that is low in the cyclone core and high near the walls has formed. Additionally, as represented in (Figures 6 and 7), the secondary vortex has formed and this is represented by the high velocity region immediately surrounding the cyclone core. If we examine the axial velocity vectors from (Figure 8) then it is clear that there is a flow reversal in the conical section of the cyclone body.

Full details of the benchmark can be found in (Tables 3-5).

5.2 Air Core Features

The air core generated in these simulations has some unique features that were unexpected. If we examine the axial volume fraction contour, (Figure 9), we can see that the air core does not completely penetrate from the overflow to the underflow. Instead it spread only partially through the body and then stopped. This state persisted indefinitely no matter how long the simulation ran for. (Delgadillo, 2005) stated that the air core which developed in his RSM simulation had a shape that was irregular and did not agree with experimental data. The shape generated in these simulations is irregular but it resembles an experimental phenomena described by (Cullivan, 2004). In that paper he shows how a quasistable air bubble persisted indefinitely for low operating pressures in the hydrocyclone.

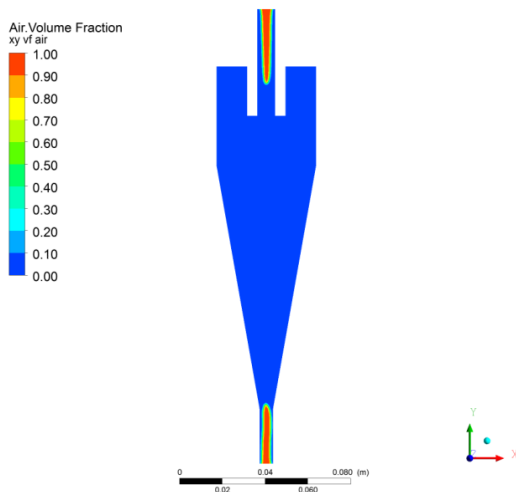
Although there was a clear low pressure region in the core of the cyclone, (Figure 10) the axial velocity at the air water interface opposes the propagation of air throughout the entire body. As evident in (Figure 10), at the overflow, the axial velocity points upwards



**Figure 7.** This figure shows the path lines that the water followed from the inlet until it exited through the underflow or overflow. From the image it is obvious that an inner and outer vortex formed as was predicted by traditional cyclone theory.

Absolute Deviation	Percent Error
Overflow (%)	Overflow (%)
17.4	20.1
13.4	15.8
17.8	20.0
13.5	16.2
16.4	19.0
Average Deviation (%)	
15.7	18.2
Standard Deviation (%)	
2.1	2.1

**Table 5.** This table shows the percent error of the simulated results at the overflow. The deviation is to be expected given the limitations of the Reynolds Stress Model.



**Figure 9.** This figure shows the volume fraction of air in the hydrocyclone after the VOF model was enabled. From this image we can tell that the air core did not completely penetrate throughout the domain but this phenomenon is similar to experimental observations by (Cullivan, 2004).

preventing the downward spread of the air core, while at the underflow the axial velocity points downwards preventing the upwards spread of the air core. Thus the air core failed to propagate through the entire body because the pressure in the center of the cyclone was not low enough to counteract the flow of water.

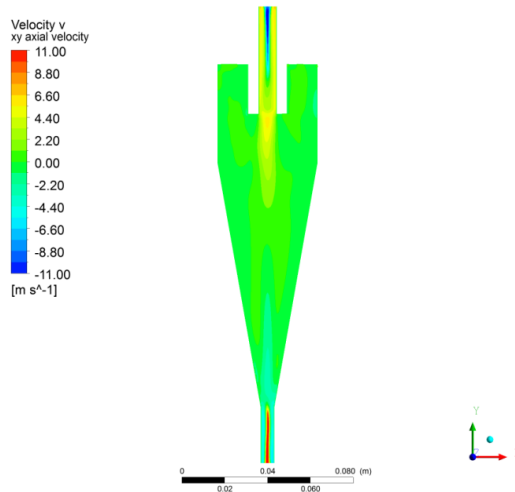
### 5.3 Particle Separation Efficiency

The particle collection efficiency of 20 $\mu$ m spherical iron particles at a flow rate of 20L/s was compared to existing commercial data to gauge the accuracy of the simulations. The simulated collection efficiency was 10% higher than the reported value. This deviation in results can be primarily attributed to the differences in flow splits between the simulation and the experiment. Since the flow split to the underflow was larger in the simulations than the experiments, we can see the reason why more particles would be collected in the simulations. While more particles overall are captured, the classification efficiency of the simulation is less than that of the real cyclone.

Additional simulations were run to compare the separation efficiency versus particle diameter but the dataset is largely incomplete. More simulations need to be run in order to generate a partition curve for this case. (Table 6) summarizes the results of the particle separation simulations; all of the simulations utilized a 20L/s flow rate.

## 6. Conclusions

The simulation model created in ANSYS FLUENT successfully captured the flow behavior of a plant hydrocyclone. A radial pressure distribution that was low in



**Figure 10.** This figure shows the velocity of the combined fluid system after the VOF model was enabled. We can see that the velocity of water at the underflow and overflow is counteracting the intrusion of air. This can help explain the failure of the air core to fully form.

the center and high near the walls formed and a flow reversal was observed in the conical section. The air core failed to completely penetrate the cyclone body but this was similar to experimental results by (Cullivan, 2004). The simulated flow split and particle separation efficiency showed reasonable agreement with reported experimental data but a future simulation utilizing the LES model is recommended. In addition, more simulations should be conducted where the dimensions of key components, such as the vortex finder or the underflow, are changed within manufacturing tolerances. The purpose of these future simulations is to determine whether the deviations in the simulated results are entirely due to the turbulence model, geometric factors, or a combination of both.

Trial	Benchmark 20 $\mu$ m	1 $\mu$ m	3.6 $\mu$ m	15.9 $\mu$ m
<b>Number of Particles</b>	139,050	27,800	27,800	27,800
<b>Particles at Overflow</b>	3	4668	2908	39
<b>Particles at Underflow</b>	138,997	22,903	24,494	27,761
<b>Did not finish</b>	50	229	398	0
<b>Collection Efficiency (%)</b>	100.0	83.1	89.4	99.9

**Table 6.** This table outlines the collection efficiency of particles at the overflow and underflow. The benchmark overestimated the collection efficiency by 10% but this could be attributed to the different flow split. We can see a trend where collection efficiency increases with particle size but more simulations are necessary to generate a complete partition curve.

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## 9. Appendix

### *Development of a Simulation Model*

Despite the simple principles behind its operation, attempts at modelling hydrocyclones have only resulted in mixed success.

(Brennan, 2009) reported that the simulated geometry has to be a close match to the actual geometry, within 5%, for the simulated data to be of any use. Slight variations in geometry, particularly with respect to the outlets and the vortex finder, result in large variations of simulation results.

Many early CFD studies of hydrocyclones simplified the cyclone model into a two dimensional grid. Although this approach simplifies the computational process greatly, research by (He, 1999; Ma, 2000; and Slack, 2000)

demonstrated the inadequacies of this simplification and the necessity of a three dimensional model.

Since the flow within the hydrocyclone is very turbulent, Reynolds Number  $\gg 4000$ , direct numerical simulations are impractical; the grid resolution requirements are on the order of  $4 \times 10^{10}$  elements. (Iaccarino, 2004) As a result, it is necessary to use a closure model to solve the Reynolds-averaged Navier-Stokes (RANS) equations.

The standard k- $\epsilon$  model struggles to account for swirling flow and previous research by (Delgadillo, 2005; Cullivan, 2003; and Slack, 2000) has shown that a second moment closure model is required. The Reynolds stress equation model (RSM) (Launder, 1975) satisfies these requirements and is the dominant turbulence closure model in hydrocyclones: RSM is utilized by (Ghodarat, 2014; Minkov, 2014; Hwang, 2013; Karimi, 2012; Brennan, 2006 & 2009; Wang, 2006; and Bhaskar, 2006) among others.

Although RSM is the dominant model used in cyclone simulations the large eddy simulation model (LES) has been reported to give better solution accuracy than RSM; however, LES requires an extremely fine grid and very small time steps to resolve all of the turbulent eddies. Each reported simulation involving LES took at least a week. (Delgadillo, 2005; Brennan, 2006; Karimi, 2012) Due to time constraints RSM was chosen for the following simulations.

Two different multiphase models are currently used to properly capture the air water interface in the center of the cyclone: the Volume of Fluid model (Hirt and Nichols, 1981) and the mixture model (Manninen, 1996) VOF was chosen for the following simulations because it was reported to generate an air core that more closely matched experimental results than the mixture model. (Karimi, 2012; Brennan, 2006)

The Discrete Phase Model (DPM) with Lagrangian particle tracking was chosen to model the particle separation efficiency because this model accurately takes into account the interactions of the particles with the continuous phase. Many previous authors have utilized the DPM, (Hwang, 2013; Murthy, 2012; Azadi, 2010; Brennan, 2009; and Delgadillo, 2007) but it has its limitations. Lagrangian particle tracking is only a valid simulation method for particle volume fractions of less than 10% because it assumes that the particles have little effect on the continuous phase. In addition, it does not take into account particle-particle interactions which affect separation efficiency at higher particle concentrations. (FLUENT Users Guide, 2012)

Image: Colored scanning electron micrograph (SEM) of a lung cancer cell.

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