Brochure



A multi-institutional regional center

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Membership

Mission

PICS is dedicated to fostering research in computational sciences in and around the Portland region. It is founded on the belief that mathematical computing has and will continue to expand scientific horizons through reliable simulations of complex phenomena and analysis of big data.

Directors

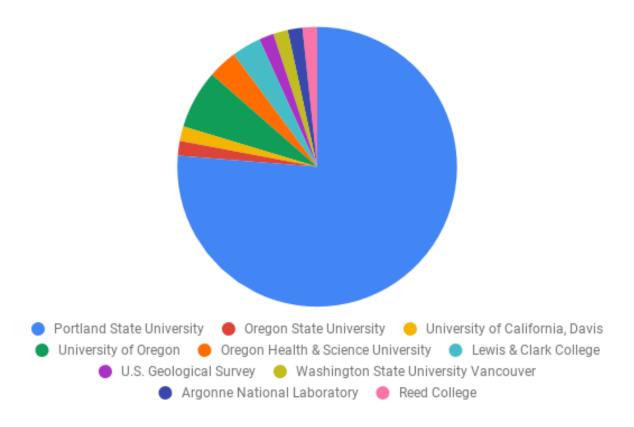
- Jay Gopalakrishnan (Maseeh Distinguished Chair & Professor, Portland State University)
- Panayot Vassilevski (Professor, Portland State University)

Types of PICS members

- 1. Stakeholders (faculty/scientists from academia/government),
- 2. Sponsored members (students/postdocs of a stakeholder),
- 3. Guest members (temporary members during a class/course).

As of September 2019, there are 216 PICS members, 58 of whom are Stakeholders.

Distribution of Stakeholders across institutions



Computational science in action at PICS

The following pages give examples of scientific advances being made by PICS members using computational techniques.

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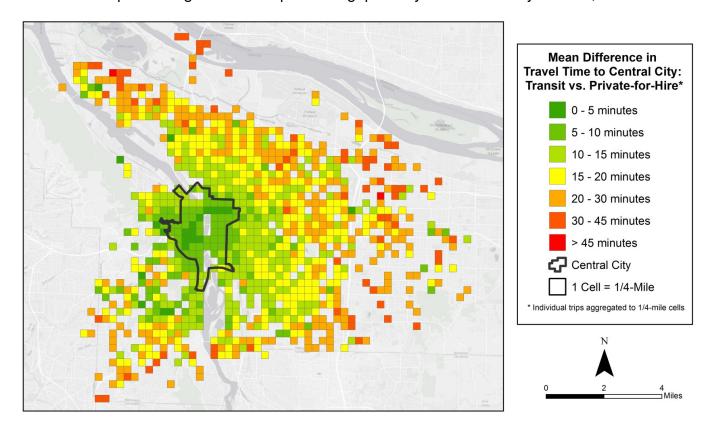
Note that these form a small subset of the ongoing activities at PICS. Please see the PICS website (pi4cs.org) for more information.



Congestion, Transit & Taxes

Private-for-Hire (PfH) transportation options, such as Uber and Lyft, are relatively new, but heavy users of transportation infrastructure in the Portland city center. PfH services also reduce Portland's mass transit userbase. How can cities maintain transportation investments and reduce congestion, while letting useful PfH concepts grow? This was the question studied by an undergraduate computational science intern, Ty Lazarchik, in the summer of 2019.

Key to anwering the question is understanding the fact that public transit options are often not competitive to PfH for trips extending far from Portland's city center, as the following figure shows. PfH options fill genuine transportation gaps away from dense city centers,



Ty's work developed an agent-based decision model in order to analyze the effectiveness of implementing a *location-based tax* in Portland city center. Computational simulations using a large number of simultaneous agents showed that implementing a low-cost location-based tax of \$1.50 would increase transit usage in the Portland area by over 1%. Projected increase in transit usage with the tax increase is catalogued in Ty's internship report [1]. Such results inform the city on potential outcomes resulting from one possible measure to encourage transit usage and reduce congestion in Portland,

PICS Members: Ty Lazarchik (REU Intern), Christof Teuscher (Faculty Mentor, Department of Electrical & Computer Engineering, Portland State University)

Reference: [1] "Modeling Changes in Public Transit and Private-for-Hire Usage When Implementing a Spatial Tax," REU Internship Report, Portland State University, 2019, Identifier: https://archives.pdx.edu/ds/psu/29397

Optical Fiber Amplifiers

Optical fiber amplifiers take signal light and amplifies it using energy from another "pump" light source by a mechanism akin to the population inversion in lasers.

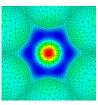
The fiber amplifier is considered one of the most revolutionary enabler of technologies in recent decades: "it has enabled our present world of long-distance ... fiber optics and ... submarine cables. The global internet could not exist as it is today without it" [1]. Outside of telecommunications, numerous other applications of fiber amplifiers have emerged: for instance, when high power is packed into ultra-thin beams of light, they can even vaporize metals – the tiny hole visible in the figure aside was created by a laser fiber amplifier.

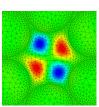
The power output of solid-state fiber laser amplifiers has been increasing over the last few decades until an unexpected roadblock was discovered, called Transverse Mode Instability (TMI). TMI refers to a sudden breakdown in the beam quality at high power operation. Theories are being put forth to explain why TMI occurs. Numerical sim-

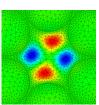


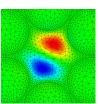
ulations can provide important insights for validating or rejecting such theories. In work supported by the Air Force Office of Scientific Research, a group of computational mathematicians at Portland State University is engaged in just that. Their hope is that the understanding gained from simulations may lead to new TMI mitigation techniques. Such simulation techniques must however be able to numerically solve the wave propagation equations within a long fiber a vast number of times, which is impractical using standard methods on current computers. In collaboration with a Dr. Jacob Grosek at the Kirtland Air Force Base, they are developing specialized numerical methods for physics-based reduced-order models utilizing the PICS supercomputing cluster extensively. The methods apply not only to the common step-index fibers, but also to the emerging photonic bandgap fibers with complex microstructures. Computed modes of one such fiber, zoomed into the fiber core region where the modes are localized, are shown below.

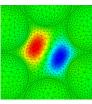


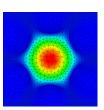












PICS Members: Dow Drake, Jay Gopalakrishnan, Tathagata Goswami, Benjamin Parker (Fariborz Maseeh Department of Mathematics & Statistics, Portland State University)

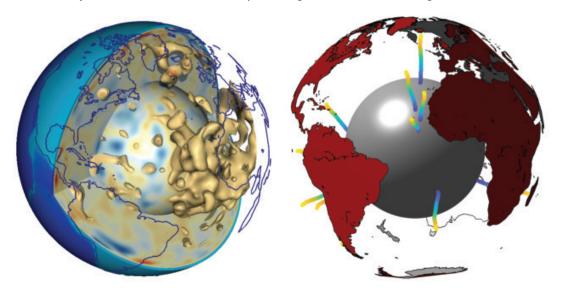
References: [1] J. Chesnoy. "EDFA Blooming" *Submarine Telecoms Forum*, 102:50–55, 2018. [2] C. Jauregui, J. Limpert & A. Tünnermann. "High-power fibre lasers." *Nature Photonics*, 7(11):861–867, 2013.



Convection in Earth's Mantle

Earth's mantle flows over timescales of thousands to billions of years. Plate tectonics and volcanoes are the surface expressions of convection within the mantle. The air that we breathe and the water in Earth's ocean have been released through volcanic degassing, so the evolution of Earth's interior is closely linked to the evolution of life and the habitability of our planet.

Geophysicist Max Rudolph at the University of California, Davis uses the PICS supercomputer to study the evolution of the structure of Earth's mantle over geologic time. Max studies fundamental questions about the dynamics of the mantle: What controls the distribution of mantle plumes in space and time? How do mantle plumes move relative to the lower mantle? How do earthquakes influence volcanic eruptions? What is the viscosity (resistance to flow) of mantle rock, and how does it affect the structure of the mantle? Modeling mantle convection is computationally challenging because of the range of length and time scales involved, from plate-boundary deformation on the scale of hundreds of meters to global-scale flow, and from timescales of thousands of years to billions of years. Additional challenges arise due to the variation of material properties and due to the uncertainty in present-day mantle structure and material properties. Max uses massively parallel computer simulations to solve the mathematical equations that govern flow in the mantle, making predictions for the development of mantle structure and the dynamics of convective upwellings and downwellings.



The above figure shows the renderings of present-day mantle structure (left) and predicted plume shapes (right) underlying presently active hotspot volcanoes. It was computed using a model of mantle convection that starts with the present-day structure of the mantle imaged using seismic waves, reconstructing mantle convection backwards through the past 75 million years, assimilating the history of tectonic plate motions.

PICS Member: Maxwell Rudolph (University of California, Davis)

References: [1] Lourenço, D.L. and Rudolph, M.L. "Shallow lower mantle viscosity modulates the pattern of mantle structure," Submitted. [2] Williams, C.D., Mukhopadyay, S., Rudolph, M.L., Romanowicz, B. "Primitive helium is sourced from seismically slow regions in the lowermost mantle," *Geochemistry, Geophysics, Geosystems* 2019, doi:10.1029/2019GC008437.

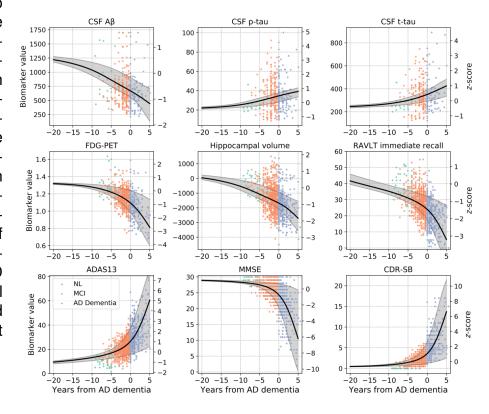


Modeling Disease Trajectory

Neurodegenerative diseases, such as Alzheimer's disease (AD), Parkinson's disease, Lou Gehrig's disease, and Huntington's disease, continue to baffle scientists despite significant research investments. One in three seniors in our country die of AD or other dementia.

A new avenue for study, of a computational nature, opened up recently when the medical community released large, comprehensive, and freely available datasets of disease progression (without identifying the patients). These rich complex datasets contain 100 to 10,000 subjects, often several visits (1 to 20) per subject, clinical and historical medical records, protein concentrations, results from MRI and molecular imaging, multiple cognitive tests, as well as genetic data. In particular, whole genome sequencing is currently available for more than 800 subjects of the ADNI (AD neuroimaging initiative) cohort. The PICS website, in an effort to contribute to reproducible research, hosts an open-ended competition for modeling the progression of AD, encouraging researchers to publish their results using a common datafreeze, which has already been downloaded many hundreds of times.

Statistics professor Bruno Jedynak at Portland State University focuses on understanding the disease progression by analyzing such datasets using the PICS supercomputer. His model provides a quantitative template of AD progression, demonstrating early changes in verbal memory, hippocampal volume loss, and cerebrospinal fluid measures of amyloid and tau. Its predictions of the onset ages of AD dementia yielded a survival curve that closely matched that of the observed onset ages (as shown aside) [1].

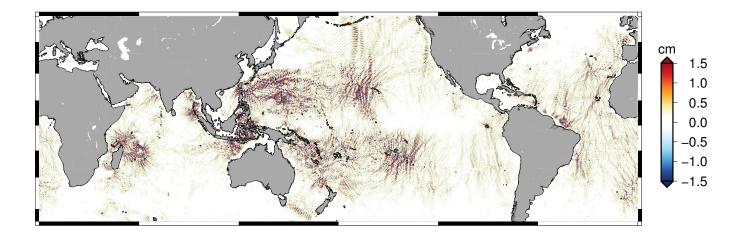


PICS Member: Bruno M. Jedynak (Fariborz Maseeh Department of Mathematics & Statistics, Portland State University)

Reference: [1] M. Bilgel and B. M. Jedynak. "Predicting time to dementia using a quantitative template of disease progression," *Alzheimer's & Dementia: Diagnosis, Assessment & Disease Monitoring*, 11:205–215, 2019.

Mapping Ocean Internal Waves

In the Department of Civil and Environmental Engineering at Portland State University, Dr. Edward Zaron is using the PICS supercomputer to map internal waves in the ocean using remotely-sensed data from NASA satellites. Satellites typically cannot measure the ocean interior, but Dr. Zaron's research is showing how the waves which propagate through the ocean interior redistribute energy and lead to transports of heat and nutrients essential to ocean life and Earth's climate. He uses the PICS supercomputer to analyze data collected by satellite radar altimeters – space-borne instruments which precisely measure small deflections of the ocean surface – to map these internal waves, showing patterns which would be impossible to measure from Earth due to the cost of obtaining global ship-based observations.



The map above was computed in a few hours using parallel computations on hundreds of processing units of the PICS cluster, a task which would take months on smaller computers. It illustrates the geographic variability of the ocean internal waves, specifically, those waves associated with the twice-per-day ocean tide. The waves are generated underwater where tidal currents push water across topographic features such as seamounts and mid-ocean ridges. Information from his research is being used to validate advanced computer models used for predicting the ocean and Earth's climate. It also has practical applications for other oceanographers studying ocean tides and internal waves.

Dr. Zaron's research is supported by three different programs at NASA, as well as the Physical Oceanography Program of the National Science Foundation. Supercomputers are essential tools in his research.

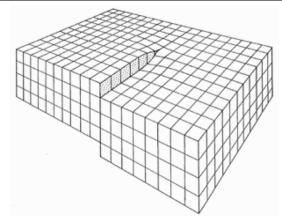
PICS Member: Edward Zaron (Civil & Environmental Engineering, Portland State University)

Reference: Zaron, E. D., "Baroclinic tidal sea level from exact-repeat mission altimetry." *J. Phys. Oceanogr.*, 49 (1), 193–210, 2019.



Dislocations in Metals

Engineer, entrepreneur, and owner of a small Portland start-up company, Dr. Saurabh Puri, had a problem: how to select what he wants from a seemingly infinite array of technical advances in computational mathematics made in academia? His company's goal is not to produce new mathematics, but rather to develop affordable computational tools for predicting microstructural evolution of dislocations and its effect on the macroscopic properties of metals. He had neither the manpower nor the time to delve into mathematics journals. So he decided to tap into the expertise of computational mathematicians at PICS.





(a) Schematic of a screw dislocation

(b) Transission electron micrograph of dislocations [1]

In crystalline metals, atoms are arranged in repeating patterns. Microscopic defects in these patterns, such as dislocations, influence the macroscopic structural properties of metals. Movement of many atomistic crystal dislocations create localized regions of high dislocation densities observable under an electron microscope (see aside). They influence the structural properties of metallic components (such as ductility, fatigue life, and failure). These properties are important in so many varied industries, that many, including Dr. Puri, are in pursuit of accurate models that can predict the evolution of dislocation patterns.

Portland State University's mathematics PhD student Dow Drake completed an internship at the company to learn more about the underlying physics and existing models. Together with his faculty advisor, he is programming cutting-edge tools for simulating the evolution of plastic distortion using advanced discontinuous Galerkin methods. In the summer of 2019, an undergraduate student from California, Kiet Tran, on internship at the Portland REU Site "Computational Modeling Serving the City" chose to be apprenticed in this project group. Together they used the PICS supercomputer extensively to perform parameter studies to gain insights into various models. New simulation tools are being produced, evaluated, and cross verified in this project, with the eventual goal of recommending the best possible computational techniques to a small business in need.

PICS Members: Dow Drake (PhD Student), Jay Gopalakrishnan (Faculty Mentor), Saurabh Puri (City Partner), Kiet Tran (REU Intern)

Reference: [1] Image from Wikipedia Commons: