NEW FRONTIERS IN LEADERSHIP COMPUTING
Training the Next Generation of Computational Geoscientists

Ker Than I School of Earth Sciences, Stanford University

A new graduate program at Stanford University trains students in the use of high-performance computing (HPC) techniques to help analyze, simulate, and predict Earth's myriad systems and interactions.

The Computational Geoscience program, or CompGeo, is a partnership between the School of Earth Sciences (SES) and the Institute for Computational Mathematics and Engineering (ICME). It is aimed at both Earth science students who want to develop expertise in computational research and students interested in computation who want to focus on problems in the geosciences. As Hamid Tchelepi noted, people are often surprised to learn that supercomputing plays a role in modern Earth sciences, but Earth scientists use more computer resources than almost anybody except the defense industry, and their computing needs can influence the design of next-generation hardware. Tchelepi is a professor of Energy Resources Engineering and co-director of Stanford's Center for Computational Energy and Environmental Science (CEES), a high-performance facility used by SES faculty.

"Earth science is about understanding the complex and ever-changing dynamics of flowing air, water, oil, gas, CO2, and heat," Tchelepi said. "That's a lot of physics, requiring extensive computing resources to model."

Tchelepi's own research involves using supercomputers to study interactions between injected CO2 gas and the complex rock-fluid system in the subsurface. "Carbon sequestration is not a simple reversal of the technology that allows us to extract oil and gas. The physics involved is more complicated, ranging from the micro-scale of sand grains to extremely large geological formations that may extend hundreds of kilometers, and the timescales are on the order of centuries, not decades," Tchelepi said.

For example, modeling how a large plume of CO2 injected into the ground migrates and settles within the subsurface, and whether it might escape from the injection site to affect the air quality of a nearby city, can require the solving of tens of millions of equations simultaneously.

Several students who study the intricate Earth system also have access to an unprecedented wealth of data gathered from different sources, ranging from satellites and aircraft-based sensors to ground-based arrays and an assortment of mobile sensors. "The amount of data that we're collecting in the Earth sciences is exploding," said Biondo Biondi, professor of Geophysics who also co-directs CEES and is the director for CompGeo. Supercomputers are playing an increasingly vital role in weavine all of these data streams together to answer important scientific questions, such as how altering atmospheric CO2 levels will affect global climate. "Computational mathematics is the backbone of modern geosciences," said ICME director Margot Gerritsen, who is also an associate professor of Energy Resources Engineering.

Through close collaborations with the computer and oil industries, and at national labs that model atmospheric and ocean patterns, Biondi knows from firsthand experience the high demand there is for professionals with the kind of training CompGeo students receive. "Potential employers repeatedly tell me that their need to hire people with these very specific sets of skills," Biondi said.

CompGeo was specifically created to address the lack at both the national and global levels of graduate programs that focus on the general interaction of computation and science. This is of particular concern in the field of computational geoscience, where there has traditionally been a lack of scientists able to fully and efficiently use advanced high-performance computational resources.

The CompGeo curriculum draws from a combination of existing courses offered at Stanford through ICME as well as many new courses in computational geoscience developed by the School of Earth Sciences. CompGeo students also have access to software and hardware at CEES. Graduates of the master's program are prepared to continue as a doctoral program or to work as scientific computing professionals in industry and government.

CompGeo student Daniel Blatter envisions computational mathematics as a key driver of geoscience discoveries for many years to come. "Whether you are interested in climate modeling or subsurface imaging, CompGeo is a great foundation for your research," he said.

Specifics

The CompGeo program is offered as a master's in science. This graduate degree track within the ICME provides students the skills and knowledge required to develop efficient and robust numerical solutions to Earth science problems using HPC. The CompGeo curriculum is based on four fundamental areas:

Modern Programming Methods for Science and Engineering

This first area focuses on object-oriented languages (C++, Fortran 2003); software development and maintenance tools; and leveraging open source software packages.

Applied Mathematics with an Emphasis on Numerical Methods

The second area focuses on partial differential equation solvers (finite difference, finite element, and finite volume); optimization algorithms (gradient-based and global); joint-state methods; and stochastic methods and computation with uncertainties.

Algorithms and Architectures for HPC

A third area focuses on large-scale parallel algorithms and tools (OpenMP, Pthreads, and message passing interface [MPI]); optimization for modern architectures (multicore, GPU, and field-programmable gate array [FPGA]); and distributed computing and large databases.

Computationally Oriented Earth Sciences Courses

The fourth and final area focuses on reservoir simulation; geophysical imaging; tectonophysics and geomechanics; climate, atmosphere, and oceans; and ecology and geobiology.

Research Areas

In addition to the curriculum areas, research can be focused in any of the departments within the School of Earth Sciences: Energy Resources Engineering; Environmental Earth System Sciences; Geological and Environmental Sciences; and Geophysics.

Academics

Now, let's take a look at the specific academic requirements.

CompGeo Requirements

As previously mentioned, the master's in science CompGeo track is offered through the ICME. For more information about the requirements and admissions process, please see the ICME website (https://icme.stanford.edu).

Students are required to take a total of 45 units of coursework and research credits to earn a degree. The coursework follows the requirements of the traditional ICME master's degree with additional requirements placed on the general and focused electives. As defined in the general Graduate Student Requirements, students must maintain a grade point average (GPA) of 3.0 or better. All courses must be taken at the 200 level or higher. To continue on to the Ph.D. program in ICME, master's students must maintain a GPA of at least 3.5.

Requirement 1: Foundational Knowledge

Students must demonstrate foundational knowledge in the field by completing the courses in two of the three core parts (see Table 1).

Courses in this area must be taken for letter grades. Deviations from the core curriculum must be justified in writing and approved by the student's ICME advisor and the chair of the ICME curriculum committee. Courses that are waived may not be counted towards the master's degree.

Requirement 2: Breadth Electives in Computational Geoscience

The master's CompGeo track requires 18 units of course work in the geosciences (three units can be applied from a non-computationally focused course). Courses are currently offered, but aren't limited to the following specific areas of the School of Earth Sciences:

- reservoir simulation;
- geophysical imaging;
- tectonophysics and geomechanics;
- climate, atmosphere, and oceans;
- and ecology and geobiology.

The Earth science courses—offered in the Environmental Earth System Science (EESS), Energy Resources Engineering (ERE), Geological and Environmental Sciences (GES), and Geophysics—Departments at Stanford—are selected based on the area of the student's interest and their research/thesis work, along with the advice and consent of the student's advisor. Students are encouraged to choose a range of courses to guarantee breadth of knowledge in Earth Sciences. A maximum of one non-computationally oriented course can be counted towards the master's degree requirements. A list of courses that fulfill these requirements is available at https://pangea.stanford.edu/programs/compgeo/academicscourses.

Requirement 3: Integrative Research in Computational Geoscience

The degree requires nine units of focused research in computational geoscience. Students are required to either...
Table 1. Foundational requirements.

<table>
<thead>
<tr>
<th>Part 1 (6 units)</th>
<th>Course number</th>
<th>Course title</th>
<th>Units per class</th>
</tr>
</thead>
<tbody>
<tr>
<td>CME 303</td>
<td>Partial Differential Equations of Applied Mathematics</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>CME 306</td>
<td>Numerical Solution of Partial Differential Equations</td>
<td>3</td>
<td></td>
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Part 2 (6 units)

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<thead>
<tr>
<th>Course number</th>
<th>Course title</th>
<th>Units per class</th>
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</thead>
<tbody>
<tr>
<td>CME 302</td>
<td>Numerical Linear Algebra</td>
<td>3</td>
</tr>
<tr>
<td>CME 304</td>
<td>Numerical Optimization</td>
<td>3</td>
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</tbody>
</table>

Part 3 (6 units)

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<thead>
<tr>
<th>Course number</th>
<th>Course title</th>
<th>Units per class</th>
</tr>
</thead>
<tbody>
<tr>
<td>CME 305</td>
<td>Discrete Mathematics and Algorithms</td>
<td>3</td>
</tr>
<tr>
<td>CME 308</td>
<td>Stochastic Methods in Engineering</td>
<td>3</td>
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</table>

Table 2. Example programs of study for computational geoscience.

<table>
<thead>
<tr>
<th>Quarter</th>
<th>Climate modeling</th>
<th>Geophysical modeling and data analysis</th>
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<tbody>
<tr>
<td>Autumn</td>
<td>EARTHSCI 310: Computational Geoscience Seminar</td>
<td>EARTHSCI 310: Computational Geoscience Seminar</td>
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<tr>
<td></td>
<td>CME 302: Numerical Linear Algebra</td>
<td>CME 302: Numerical Linear Algebra</td>
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<td></td>
<td>CEE 262A: Hydrodynamics</td>
<td>CEE 262A: Hydrodynamics</td>
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<tr>
<td>Winter</td>
<td>CME 212: Advanced Programming for Scientists and Engineers</td>
<td>CME 212: Advanced Programming for Scientists and Engineers</td>
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<td></td>
<td>EESS 245A: Atmosphere, Ocean, and Climate Dynamics</td>
<td>EESS 245A: Atmosphere, Ocean, and Climate Dynamics</td>
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<td></td>
<td>The Atmospheric Circulation</td>
<td>The Atmospheric Circulation</td>
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<tr>
<td>Spring</td>
<td>CME 213: Introduction to Parallel Computing Using MPI, Open MPI, and CUDA</td>
<td>CME 213: Introduction to Parallel Computing Using MPI, Open MPI, and CUDA</td>
</tr>
<tr>
<td></td>
<td>EESS 246A: Atmosphere, Ocean, and Climate Dynamics</td>
<td>EESS 246A: Atmosphere, Ocean, and Climate Dynamics</td>
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<td></td>
<td>EARTHSCI 400: Directed Research</td>
<td>EARTHSCI 400: Directed Research</td>
</tr>
<tr>
<td>Summer</td>
<td>EARTHSCI 400: Directed Research</td>
<td>EARTHSCI 400: Directed Research</td>
</tr>
<tr>
<td>Autumn</td>
<td>EARTHSCI 310: Computational Geoscience Seminar</td>
<td>EARTHSCI 310: Computational Geoscience Seminar</td>
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<tr>
<td></td>
<td>ECE 262B: Transport in Surface Water Flows</td>
<td>ECE 262B: Transport in Surface Water Flows</td>
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<td>E grave 262A: Hydrodynamics</td>
<td>E grave 262A: Hydrodynamics</td>
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<tr>
<td></td>
<td>CET 262D: Introduction to Computational Earth Sciences</td>
<td>CET 262D: Introduction to Computational Earth Sciences</td>
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<tr>
<td></td>
<td>CET 262B: Transport in Surface Water Flows</td>
<td>CET 262B: Transport in Surface Water Flows</td>
</tr>
<tr>
<td></td>
<td>CET 262A: Hydrodynamics</td>
<td>CET 262A: Hydrodynamics</td>
</tr>
</tbody>
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**Environmental/Climate/Hydrogeology**
- EESS 215: Earth System Dynamics
- EESS 220: Physical Hydrogeology
- EESS 231: Contaminant Hydrogeology
- EESS 246B: Atmosphere, Ocean, and Climate Dynamics
- EGS 224: Modeling Transport and Transformations in the Environment
- EGS 264: Mathematical Modeling in Biogeochemistry

**Geophysical Imaging**
- GEOPHYS 204: Spectral Finite Element Method Seismograms
- GEOPHYS 210: Basic Earth Imaging
- GEOPHYS 211: Environmental Soundings Image Estimation
- GEOPHYS 240: Borehole Seismic Modeling and Imaging
- GEOPHYS 280: 3D - Seismic Imaging
- GEOPHYS 287: Earthquake Seismology

**General Computational/Mathematical Geoscience**
- EESS 214: Introduction to Geostatistics and Modeling of Spatial Uncertainty
- EESS 260: Advanced Statistical Methods
- EESS 260: Modeling Uncertainty in the Earth Sciences
- EGS 244: Optimization of Energy Systems
- EGS 284: Optimization and Inverse Modeling
- GEOS 240: Geostatistics
- GEOPHYS 258: Scientific Data Processing
- GEOPHYS 281: Geophysical Inverse Problems

**Reservoir Simulation/Fluid Flow**
- GEOPHYS 200: Fluid and Flow in the Earth: Computational Methods
- EGS 275: Quantitative Methods in Basin and Petroleum Systems Modeling
- EGS 275: Reservoir Simulation
- EGS 275: Advanced Reservoir Simulation
- EGS 275: Applied Mathematics in Reservoir Engineering
- EGS 275: Numerical Modeling of Fluid Flow in Porous Media

**Subsurface and Reservoir Characterization**
- GEOPHYS 202: Reservoir Geomechanics
- GEOPHYS 241: Seismic Reservoir Characterization
- GEOPHYS 260: Rock Physics for Reservoir Characterization

**Structural/Tectonophysics/Geomechanics**
- GEOPHYS 220: Ice, Water, Fire
- GEOPHYS 251: Structural Geology and Rock Mechanics
- GEOPHYS 289A: Crustal Deformation
- GEOPHYS 290: Tectonophysics

**Figure 1.** A sample of computational geosciences courses offered in the School of Earth Sciences. (ENERGY = Energy Resources Engineering; EESS = Environmental Earth System Science; GES = Geological and Environmental Sciences; and GEOPHYS = Geophysics.)

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