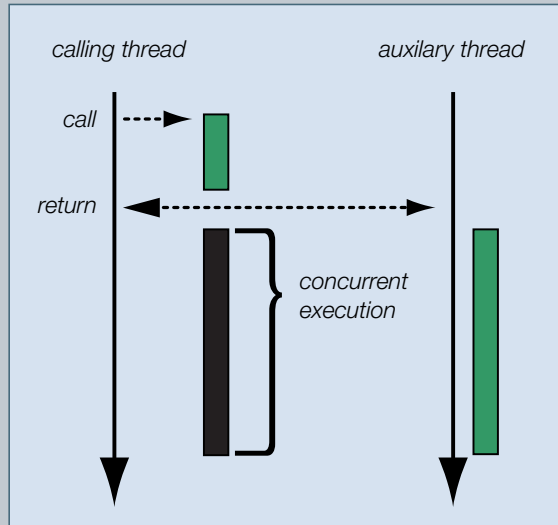
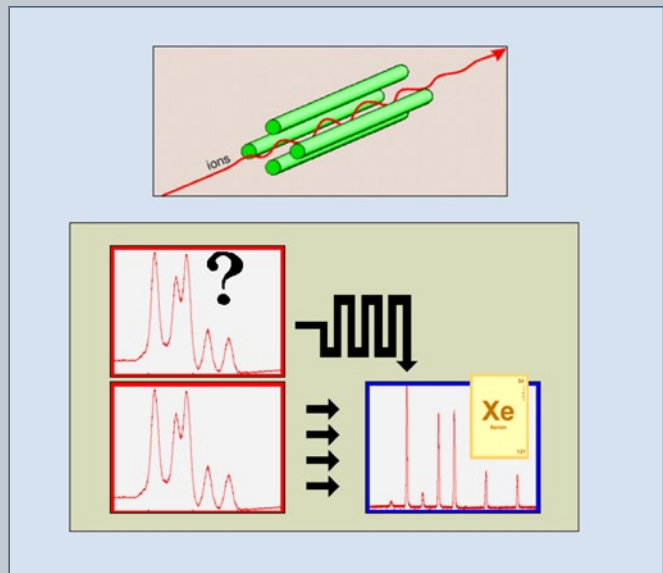


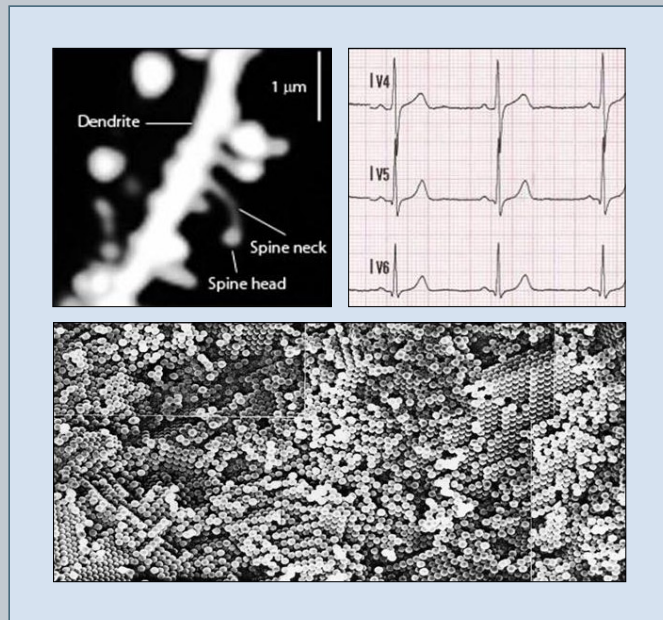
# High-Performance and Scientific Computing



SwRI researchers design and implement software and programming models that enable highly parallel systems, reducing the need for users to be aware of complex multicore architectures.



Using OpenMP, SwRI accelerated quadrupole MS data deconvolution and library matching.



SwRI provides engineering expertise to increase speed and fidelity of existing scientific computing codes.

Southwest Research Institute® (SwRI®) is working to enhance the state of the art in high-performance computing and apply new technologies to scientific computing applications.

## High-Performance Computing

The high-performance computing field has shifted focus to multi-core CPU (central processing unit) designs that achieve faster execution times by performing tasks in parallel, which has been the favored approach in GPU (graphics processing unit) design. Additionally, CPU and GPU architectures have begun to converge in advanced GPGPU (general-purpose computation on GPU) architectures.

SwRI has experience in implementing and optimizing applications using multicore and GPGPU techniques such as:

- Enabling parallelism within applications using OpenMP and MPI
- Executing code on GPGPUs using CUDA
- Using OpenCL to enable source portability
- Optimizing critical sections using assembly language

## Scientific Computing

SwRI has a unique combination of advanced capabilities in computer engineering coupled with extensive expertise in a variety of physical sciences. Recent efforts have optimized applications including:

- Computational fluid dynamics (CFD) simulation of water flow
- Utilization of computational chemistry to model and predict chemical reactions
- Identification of unknown compounds using mass spectroscopy

SwRI has deep expertise in languages commonly used for scientific computing including:

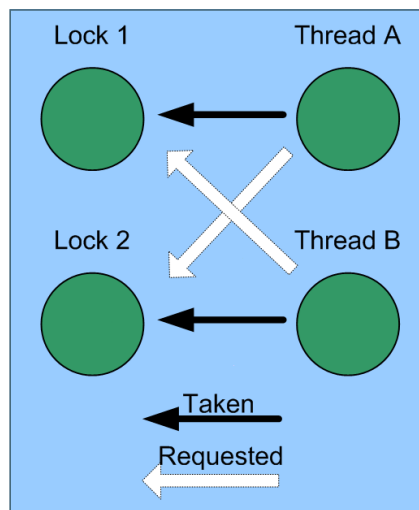
- Fortran
- C/C++
- Python

## Advanced Application Programming Interfaces and Compiler Tools

Application programming interfaces (APIs) and compiler tools developed at SwRI enable both data and task parallelization while remaining free of race and deadlock conditions. Low-level concurrency primitives can be hidden from the developer to reduce program complexity and facilitate rapid development of parallel programs.

SwRI's approaches to simplifying development include:

- Template-based generic programming
- Static source code analysis and transformation



$$\frac{1}{(1 - P) + \frac{P}{S}}$$

SwRI researchers use advanced parallelization techniques to manage concurrency, avoid deadlock, and maximize speedup.



*Southwest Research Institute is an independent, nonprofit, applied engineering and physical sciences research and development organization using multidisciplinary approaches to problem solving. The Institute occupies 1,200 acres in San Antonio, Texas, and provides more than 2 million square feet of laboratories, test facilities, workshops and offices for more than 3,200 employees who perform contract work for industry and government clients.*

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