# Denoising of Signals from Electron Spin Resonance Machines

CAC

## Project description

The National Biomedical Center for Advanced ESR Technology (ACERT) is located at Cornell University and is supported by the National Institute of General Medical Sciences (NIGMS), part of the National Institutes of Health. One of the areas of Technology R&D at ACERT is improving the computational methods used for Electron Spin Resonance (ESR) analysis and spectral processing. ACERT is in a unique position to make these improvements because of the extensive Driving Biomedical Projects and collaborative/service projects at the Center. These projects are aimed at understanding and combating diseases and ailments such as Alzheimer's, cancer, depressive disorders, Parkinson's, and SARS by studying their key proteins' structure and functional mechanisms. Despite major advances in biophysical techniques such as ESR, NMR, MRI and cryo-EM, physical methods lack sufficient sensitivity and resolution to conduct biological studies in native conditions, primarily due to the presence of experimental noise. To separate experimental signals from noise, Madhur Srivastava and colleagues in his Signal Science Lab developed a wavelet-based denoising of signals technique that localizes and removes noise from signals, especially when the noise is dominant.

## CAC services

To deploy this technique and make his software vision a reality, Srivastava decided to collaborate with the Cornell Center for Advanced Computing (CAC). Senior research associate Chris Myers developed a webserver that supports the denoising of signals, as well as the reconstruction of auxiliary data based upon those denoised signals. The webserver runs on Red Cloud, an Infrastructure as a Service cloud located on Cornell's Ithaca campus. At present, three different applications are running on Red Cloud to support the computational workflows. Myers took prototype MATLAB code, provided by Srivastava, that implements the core numerical operations, and then implemented Python-based numerical applications with graphical front-ends built using the Bokeh library for interactive web-based graphics and visualization. CAC senior research associate Steve Lantz and cloud systems engineer Bennett Wineholt were instrumental in working with Myers to flesh out the original webserver design and to implement key pieces of the server-side configuration that supports the Python/Bokeh applications that carry out the data processing. Nginx was chosen as the security layer between the users and the applications.

## Results

Srivastava's methodology and research performed by Engaged Cornell undergraduate students has gained the attention of the magnetic resonance community. He has given over 17 invited talks, including the 62nd Experimental Nuclear Magnetic Resonance Conference where he explained how the wavelet transform-based approach effectively removes noise for spectroscopic data. Srivastava, along with Cornell professors Jack H. Freed and C. Lindsay Anderson, also submitted a US Patent application for this technique titled "Systems, Methods, and Programs for Denoising Signals Using Wavelets." "The fact that these applications are running on CAC's webserver spares our users from having to install a number of software packages locally on their own machines," says Srivastava. "It also means our users can access the latest software packages as they are deployed." Myers and Lantz provided in-person support for an ACERT Workshop that introduced the new methodology. Myers continues to work with Srivastava to add new features to the software, requested either by him, or increasingly, by other users.

CLIENT

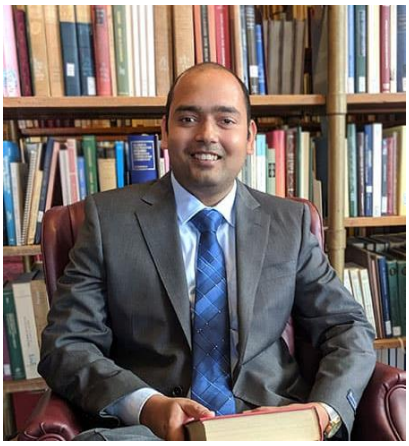
ACERT

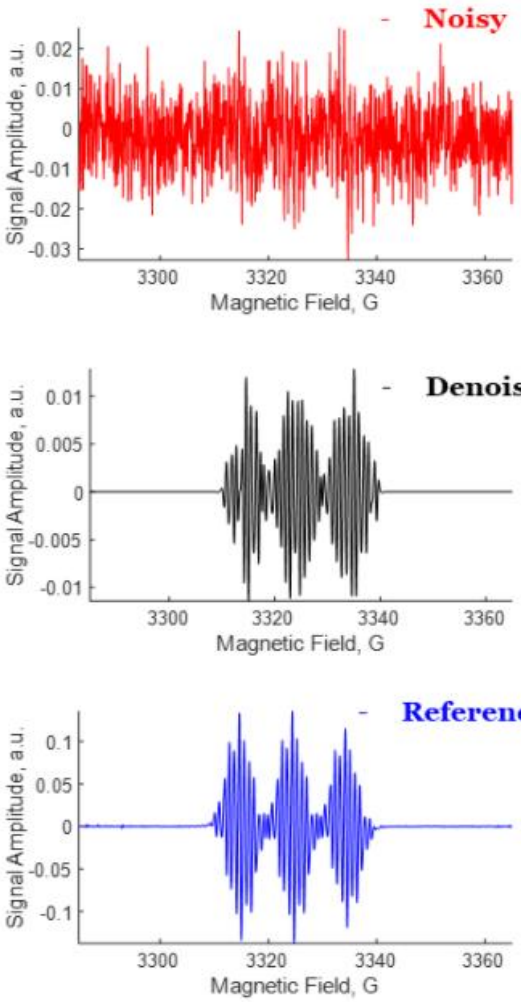
Madhur Srivastava

Cornell Chemistry & Chemical Biology

SERVICES

- Python Programming
- Server Configuration
- Red Cloud Computing
- Web Interface
- Data Visualization




*To overcome noise problems in physical methods, Madhur Srivastava's Signal Science Lab is developing wavelet transform-based noise reduction algorithms that include multi-dimensional representation of signals, development of customized wavelets, enhancement in signal resolution in the wavelet domain, and development of noise thresholds.*

Besides research in wavelet denoising, the Signal Science Lab is leading efforts to develop fundamental data processing methods and advanced computational workflows to extract high-fidelity signals with excellent spatial and temporal resolution from physical measurements. "We look forward to continued collaborations with CAC," says Srivastava. "Their software, data, and computing skills are enabling new insights while enhancing the productivity of our users."

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ABOUT CAC

The Cornell University Center for Advanced Computing is located in Ithaca, NY. With a professional staff of computational and data scientists, cyberinfrastructure specialists, and a breadth of PhD-level expertise in astronomy, biology, computer science, information science, mathematics, and physics, CAC is creating tomorrow's software, data and computing solutions today.

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