**Prof. Goran Neshich**
Computational Biology Research Group - Embrapa Agricultural Informatics

**Title of the talk:**
**"BlueStar STING platform for analysis of protein structure / function relationship: Designing agrochemicals to fit new protein targets for bacterial, fungal and insect control"**

Blue Star STING suite of programs for comprehensive analysis of structure, function and stability of proteins and their complexes, has matured over a decade of development. We will present the in silico process for identification of the catalytic site amino acids by means of selecting a range for values for a set of the STING_DB parameters - protein structure descriptors. Also, we developed a new hydrophobicity index which we now use for characterization of protein interfaces - details of which will be discussed within specific biological problems. Specific applications in agriculture and medicine will also be mentioned and discussed with emphasis on diseases such as the Amyotrophic lateral sclerosis (ALS), also called motor neuron disease, is a progressive paralytic disorder that is usually fatal within some years of onset of symptoms. The paralysis is due to degeneration of large motor neurons of the spinal cord, brainstem and motor cortex. About 10% of ALS cases are Familial ALS (FALS), and of these, around 25% are linked to mutations in sod1, the gene encoding Cooper/Zinc Superoxide Dismutase (SOD1). More than 90 FALS-linked SOD1 mutations have been discovered, and the Ala4Val (A4V) mutant is the most common revealed to date, accounting for ≈50% of SOD1-linked FALS cases.What we found with the help of MSSP module of BlueStar STING is that residues in mutated protein that are engaged in coordination of metal ions do show a very different Electrostatic Potential characteristics and this fact may well explain the changing in state of metal ion coordination which can lead to observed phenotype.