Departamento de Informática – UTFSM

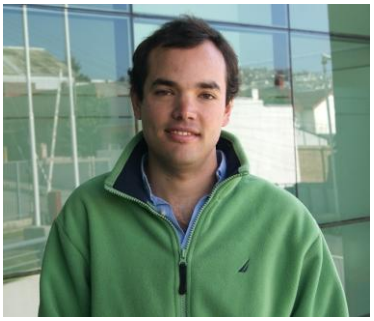
Ciclo de Coloquios 2015

El Departamento de Informática de la Universidad Técnica Federico Santa María tiene el agrado de invitar a la comunidad universitaria a su tercer coloquio departamental. La presentación se realizará en el Auditorio Claudio Matamoros (F-106), Casa Central, el día **martes 31 de Marzo a las 12:00** y por videoconferencia al Laboratorio de Programación Avanzada, Departamento de Informática, Campus San Joaquín, UTFSM.

Título

Biomolecular electrostatics with continuum models:
a boundary integral implementation and applications to biosensors

Invitado



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Mini Bio

Christopher Cooper es instructor académico del Departamento de Ingeniería Mecánica de la Universidad Técnica Federico Santa María desde marzo del año 2015. Él es ingeniero mecánico de la misma casa de estudios (2009), y obtuvo un MS (2012) y un PhD (2015) en ingeniería mecánica de Boston University. Su área de investigación es la simluación numérica de fenómenos físicos, con aplicaciones en electrostática molecular y mecánica de fluidos.

Resumen

The implicit-solvent model uses continuum electrostatic theory to represent the potential around biomolecules dissolved in a salt solution. This leads to a system of PDEs where the Poisson-Boltzmann and Poisson equations are coupled on the molecular surface. To solve the resulting system of PDEs efficiently, we wrote a fast boundary-element method (with a multipole-based treecode) in Python and CUDA (for exploiting GPUs). We call our code PyGBe --- a Python-based GPU code for boundary elements. We will show results that verify and validate our implementation of PyGBe in the context of solvation and binding of biomolecules, comparing it with experimental observations, analytical solutions, and other numerical tools.
Our main application of interest looks at the preferred orientation of proteins adsorbed on a charged surface, a situation relevant in biosensing. Biosensors are designed to detect a target molecule when it binds to a ligand molecule, itself attached to the sensor through a self-assembled monolayer (SAM). It is key that the binding sites of the ligand molecule be adequately exposed to the flow that carries the targets, and hence the importance of orientation. In our model, surfaces with SAMs are represented by prescribing a charge distribution.
We will present results for three test cases of adsorption. The first case is used to verify the code; it compares the numerical result with an analytical solution derived by us, valid for a spherical surface interacting with a spherical protein with a centered charge. In the second case, we used PyGBe to compute the preferred orientation for protein G B1 adsorbed on a charged surface and compared the result with published molecular dynamics (MD) simulations and experimental observations, matching the preferred orientation. In the third and final case, we used a full antibody, a common ligand molecule in biosensors that is much larger than protein G B1 and would be difficult to simulate with MD. This test shows the capability of our code to compute realistic systems for bionsensing applications.

Lugar y Fecha

31 de Marzo de 2015, 12:00
Auditorio Claudio Matamoros (F-106).
Departamento de Informática, Valparaíso. UTFSM

La charla se transmitirá en videoconferencia al laboratorio LPA,
Departamento de Informática, San Joaquín, UTFSM.