UNIVERSIDAD TECNICA
FEDERICO SANTA MARIA

DEPARTAMENTO DE INGENIERÍA MECÁNICA

CHARLA

En el marco de la asignatura Seminario de Ingeniería Mecánica, se invita a la Comunidad Universitaria a participar de la Charla:

"Continuum models at nanoscale: electrostatics in molecular solvation"

Expositor: Ph.D. Christopher Cooper V.

FECHA : Jueves 09 de mayo de 2019.

Hora : 11:30 hrs.

Lugar : Auditorio Pedro Roth (C-259)

– Casa Central / Valparaíso
Av. España 1680
Fono (56-32) 2 654162 / 2 654362

– Campus Santiago / San Joaquín
Avda. Vicuña Mackenna 3939
Fono (56-2) 2 4326627

UNIVERSIDAD TECNICA
FEDERICO SANTA MARIA

DEPARTAMENTO DE INGENIERÍA MECÁNICA

Continuum models at nanoscale: electrostatics in molecular solvation

Presented by: Christopher Cooper Villagrán, Ph.D.

Universidad Técnica Federico Santa María, Mechanical Engineering Department, Valparaíso, Chile.

Abstract

Electrostatics plays a key role in molecular solvation, making it important to have an appropriate treatment of the solvent. Even though these problems are usually addressed with explicit solvent models, through molecular dynamics, an implicit representation using continuum electrostatics offers an efficient, and accurate, alternative for solvation energy calculations. In particular, continuum electrostatic theory yields a system of partial differential equations in a domain that is divided into two regions (solute and solvent), with the Poisson equation governing the electrostatic potential inside the solute, and the Poisson-Boltzmann equation in the solvent, to account for mobile ions. We formulate the system of differential equations in integral form, where the integral runs on the molecular surface, and solve it with a treecode-accelerated boundary element method.

In this talk, we will discuss the advantages and disadvantages of a boundary-integral-based implicit solvent model, and show results of this approach in different biomolecular applications, such as solvation, binding, protein-surface interaction, among others. Even though the physical problems are in the nanoscale regime, we will see that the continuum approximation yields an accurate model.

Academic Experience

Académico del Departamento de Ingeniería Mecánica, Universidad Técnica Federico Santa María, Chile

Doctor of Philosophy (Ph.D.) in Mechanical Engineering, Boston University, USA

Ingeniero Civil Mecánico, Universidad Técnica Federico Santa María, Chile

Current research projects

"Preparación y caracterización de metamateriales magnéticos para detección remota de tensiones en neumáticos", FONDEF IDeA en Dos Etapas ID16I10048, 2 años, 2017, Co-investigador

"Full viruses on your local cluster: parallel simulations of virus-cell electrostatic interactions", FONDECYT Iniciación 11160768, 3 años, 2016, Investigador Principal

"Modelación y diseño de prototipo para medir tensiones en comósitos poliméricos", Proyecto Interno DGIP-USM, 1 año, 2016, Investigador Principal

"Dinámica del escurrimiento sobre una superficie porosa: aplicación a la predicción de aluviones", Proyecto Interno DGIP-USM, 1 año, 2016, Co-investigador

"Modelación numérica de moléculas ligando en biosensores", Proyecto Interno DGIP-USM 25-15-32, 1 año, 2015, Investigador Principal