# הטכניון – מכון טכנולוגי לישראל הפקולטה להנדסת מכונות



## TECHNION – Israel Institute of Technology Faculty of Mechanical Engineering

#### SEMINAR - סמינר

הנך מוזמן/ת להרצאה סמינריונית של הפקולטה להנדסת מכונות, שתתקיים ביום בי 18.07.16 (יבי בתמוז, תשעייו), בבניין דן-קאהן, קומה 0, אודיטוריום 1, 30 .14:

<u>ירצה:</u>

#### Dr. Gaddiel Ouaknin

Department of Mechanical Engineering University of California Santa Barbara, USA

על הנושא:

### **Level set Strategy for SCFT**

The seminar will be given in Hebrew

#### <u>להלן תקציר ההרצאה:</u>

This thesis investigates the design of sharp interface level set methods in the context of self-consistent field theory (SCFT) in polymer physics. SCFT computes the structure and energy of inhomogeneous self-assembling polymers at thermodynamic equilibrium. Level set methods are based on an implicit representation of free boundaries, which enable motions with arbitrary change in topology. In addition, recent advances on how to impose Robin boundary conditions enables the study of free boundary problems of interest in the community interested in self-assembly.

We first present a computational framework, encoded on a forest of quad/oct-trees in a parallel environment. We then present results of imposing sharp Neumann boundary conditions as was first proposed by de Gennes, which enables SCFT computations of meaningful quantities at the boundary of irregular geometries. We then introduce the concept of functional level-set derivative in the context of SCFT and rigorously derive expressions for the change of energy of a diblock copolymer with respect to an enclosing shape. The level-set derivative is then used to embed SCFT into a variable shape simulator, where the internal structure and the enclosing shape are coupled together and evolve in tandem in order to reduce the energy of the diblock copolymer. Finally an algorithm for solving the inverse problem for directed self-assembly is presented.

המארח: פרופי פנחס בר-יוסף

בברכה,

מרכז הסמינרים מרכז הסמינרים