山形大学グリーンマテリアル成形加工研究センター

&

YU-COE(S)ソフトマテリアル創製研究拠点

第６３回合同セミナーのお知らせ

本講演会は、対面およびビデオ会議ツール「Zoom」を使ったハイブリッド形式で行います

タイトル：

Field Theories and Molecular Representation:

Efficient Models for Large Scale Parallel MD Simulations

講演者　：　Università degli Studi di Napoli Federico II (ITALY)

Prof. Giuseppe Milano

要　旨　：

Before the scientific presentation, I will show an outline of my new affiliation including a description of teaching programs in Materials Engineering, Biomaterials Engineering, Chemical Engineering and the PhD program. In recent years, the success of modelling in understanding the fundamentals of complex molecular phenomena has triggered a strong desire to go beyond the limitations of the information that can be extracted from classical Molecular Dynamics, especially the limitations that cannot be resolved by advances in computational efficiency. To this aim, effective molecular representations have been developed and used for diverse molecular systems in a variety of coarse-grained (CG) and multi-scale (MS) techniques. (For a recent review and perspective, see [1]) In the last decade, hybrid particle-continuum approaches such (hPF-MD),[2,3] which link discrete (particle-based) and continuum (field-based) descriptions in a single simulation volume, have been increasingly applied and validated for different systems. The hPF-MD model has been demonstrated to be effective to investigate homopolymers and block copolymers at both CG[4] and atomistic resolutions [5] also in the presence of solid nanoparticles [6-9]. Many other systems (especially biomolecules) and problems can be solved by using this efficient simulation technique implemented in the massively parallel software OCCAM in a new optimized version [10].

Ref［*1*］—［*10*］については次ページ参照

日　時　：　　2022年 6月7 日 (火)　13 時 00 分～14 時 30 分

場　所　：　　GMAP　4－406

参加をご希望の方は、**事前にメールで**ご連絡をお願い致します。

伊藤・石神研究室秘書　渡辺（wkazumi@yz.yamagata-u.ac.jp）

後日、講演会参加のオンライン配信 Zoom 会議のリンク先（ミーティング ID、パスコード）をご連絡致します。
講演は対面およびオンライン配信で行います。

世話人　：　　有機材料システム　伊藤浩志　（内線 3081）

Yamagata University

Research Center for GREEN Materials and Advanced Processing &

YU-COE(S) Soft Materials Research Centre

Announcement of the 63rd Joint Seminar

This seminar will be held in a hybrid format using face-to-face and video conferencing tool "Zoom".

Date: 7 June 2022 (Tuesday) 13:00-14:30

Place: GMAP 4-406

Title : Field Theories and Molecular Representation: Efficient Models for Large Scale Parallel MD Simulations

Presenter : Prof. Giuseppe Milano,

Università degli Studi di Napoli Federico II (ITALY)

Abstract :

Before the scientific presentation, I will show an outline of my new affiliation including a description of teaching programs in Materials Engineering, Biomaterials Engineering, Chemical Engineering and the PhD program. In recent years, the success of modelling in understanding the fundamentals of complex molecular phenomena has triggered a strong desire to go beyond the limitations of the information that can be extracted from classical Molecular Dynamics, especially the limitations that cannot be resolved by advances in computational efficiency. To this aim, effective molecular representations have been developed and used for diverse molecular systems in a variety of coarse-grained (CG) and multi-scale (MS) techniques. (For a recent review and perspective, see [1]) In the last decade, hybrid particle-continuum approaches such (hPF-MD),[2,3] which link discrete (particle-based) and continuum (field-based) descriptions in a single simulation volume, have been increasingly applied and validated for different systems. The hPF-MD model has been demonstrated to be effective to investigate homopolymers and block copolymers at both CG[4] and atomistic resolutions [5] also in the presence of solid nanoparticles [6-9]. Many other systems (especially biomolecules) and problems can be solved by using this efficient simulation technique implemented in the massively parallel software OCCAM in a new optimized version [10].

See next page for Refs [1]-[10].

If you wish to attend, please contact us in advance by e-mail. Ito & Ishigami Laboratory Secretary, Ms. R. Yamaguchi (y-reiko@yz.yamagata-u.ac.jp)

We will later contact you with the link (meeting ID and passcode) for the online Zoom meeting for participation in the lecture. Lectures will be delivered in person and via online distribution.

Coordinator: Hiroshi Ito, Organic Materials Science & GMAP (ext. 3081)

References

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[3] Hybrid Particle-Field Molecular Dynamics Simulations: Parallelization and Benckmarks Y. Zhao, A. De Nicola, T. Kawakatsu, G. Milano Journal of Computational Chemistry 2012, 33, 868

[4] Micellar Drug Nanocarriers and Biomembranes: How do they Interact? A. De Nicola, S. Hezaveh, Y. Zhao, T. Kawakatsu, D. Roccatano, G. Milano Phys. Chem. Chem. Phys. 2014, 16, 5093

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[10] Efficient Hybrid Particle-Field Coarse-Grained Model of Polymer Filler Interactions: Multiscale Hierarchical Structure of Carbon Black Particles in Contact with Polyethylene Stefano Caputo, Velichko Hristov, Antonio De Nicola, Harald Herbst, Antonio Pizzirusso, Greta Donati, Gianmarco Munaò, Alexandra Romina Albunia and Giuseppe Milano J. Chem. Theory Comput. 2021, 17, 3, 1755