



# The Hong Kong Polytechnic University Department of Applied Mathematics

# Colloquium

# Model Reduction Techniques in Computational Materials Sciences

by

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#### **Abstract**

In this talk, I will illustrate the model reduction techniques through some typical issues in computational materials science, namely the temperature effects and boundary conditions. In the temperature effect issue, I will introduce our recent progress on simplifying massive molecular dynamics simulations into a direct finite dimensional algebraic calculation. In the boundary conditions issue, I will introduce an efficient and easy way to implement boundary condition for molecular dynamics simulations.

Date: 23 April, 2020 (Thursday)

Time: 2:00p.m. – 3:00p.m. Venue: Online Talk via Zoom \* The Talk will be given in English.

\*\*\* ALL ARE WELCOME \*\*\*