

# COMPUTATIONAL RESEARCH IN BOSTON AND BEYOND SEMINAR

Friday, November 1, 2024

12:00 PM – 1:00 PM

<https://mit.zoom.us/j/96155042770>



Adaptive computing: high resolution simulation at  
low resolution cost

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## Abstract:

Adaptive computing (AC) methods leverage a surrogate model to resolve small scale processes over a large-scale domain. We consider solar cell modeling, which requires coupling a fluid dynamical model for gas flow with a molecular-scale Kinetic Monte Carlo (KMC) model for the development of perovskite crystal lattices. Within each grid cell of the boundary layer, the fluid dynamical driver uses the AC framework to determine lattice formation. The AC framework determines when to call the KMC code or use the computationally inexpensive surrogate model estimate. We present two approaches using different constraints. First, a computational budget fixes the number of KMC model runs while minimizing uncertainty in the surrogate model training. Second, an accuracy budget limits uncertainty in the result while maximizing use of the surrogate.

<https://math.mit.edu/crib/>