Canadian Association
of Physicists

Association canadienne
des physiciens et physiciennes

Contribution ID: **3678**   Type: **Invited Speaker / Conférencier(ère) invité(e)**

(I) Neural-network-based solver for a few soft matter problems

Monday 19 June 2023 16:45 (30 minutes)

Many soft matter theoretical problems can be reformulated into minimizing a cost function, in which the field-based physical properties (the target functions) are adjusted to achieve the minimum. The Neural-network approach approximates the target functions by forward-feeding neural networks and the machine-learning techniques adjust the network parameters to produce the approximation to the desirable solutions. The physical properties, such as the free energy, together with boundary conditions, etc, are modelled in the cost function. The decoupling between the function approximator and sampling space allows for further incorporation of the weighted Monte Carlo method. The algorithm is demonstrated here by solving a few classical theoretical problems in soft matter.

Keyword-1

Soft Matter

Keyword-2

Neural Network

Keyword-3

Computer simulation

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Session Classification: (DCMMP) M3-7 Soft Condensed Matter II | Matière condensée molle II (DPMCM)

Track Classification: Technical Sessions / Sessions techniques: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)