Phase behaviour of a 2D system exhibiting inverse melting[1]
AHMAD ALMUDALLAL, Memorial University of Newfoundland, SERGEY BULDYREV, Yeshiva University, IVAN SAIKA-VOIVOD, Memorial University of Newfoundland — We calculate the phase diagram for a square-shoulder square-well potential in two dimensions using Monte Carlo simulation techniques. This potential has been previously used as a model for understanding the connection between the anomalous properties of liquid water and a hypothesized metastable liquid-liquid critical point. In our phase diagram, we find that melting lines appear to be first order, and that one of them exhibits a maximum temperature as well as a maximum pressure, indicating inverse melting (crystallization upon heating) over a small range in pressure. We apply Hamiltonian Gibbs-Duhem integration to find potential parameters that maximize the pressure range over which inverse melting occurs.

Ahmad Almudallal
Memorial University of Newfoundland