ORDER PARAMETERS FOR DETECTION AND DEMARKATION OF INTERFACES IN HYDRATE-FLUID AND ICE-FLUID SYSTEMS

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ABSTRACT
This article contains 6 sections. The first section gives a brief description of the models and the system used. In the second section the order parameters are defined and discussed with focus on interface demarcation. In section three the melting temperatures of the phases are estimated. In the forth and fifth section the hydrophilic/hydrophobic interfaces hydrate II/oil and ice-Ih/oil and hydrophilic/hydrophilic interfaces: hydrate/water and ice/water are discussed focussing on the influence of the spatial and temporal sampling rates and filtering on the quality of the order parameter field. The precision of each order parameter is studied together with the correlations between them in comparable cases. In the sixth section, the quality of the results in the fourth and fifth sections for interface demarcation is assessed. The last section is the conclusion with a brief discussion of the feasibility of using this approach with the Surface Fluctuation method to quantify the energetics of the interfaces.

Keywords: Ice, hydrates, liquid, interface demarkation, order parameter

SYSTEM CONFIGURATION
Molecular Models
The 4-site TIP4P/ice water model [1] was used, the OPLS-UA parameters for the Propane guest molecules in the hydrate phase, and the OPLS-AA forcefield for the liquid oil phase (which consisted of octane molecules).

Geometric configurations
Two solid phases, denoted by A, and three fluids, denoted by B, were used. Previous work using the capillary wave method on single Lennard-Jones-spheres have used a rectangular slab geometry with an B-A-B (or A-B-A) configuration. Two different geometries have been proposed, the quasi-1D strip [10, 5] ge-