Molecular Thermodynamics: Towards a generic strategy to develop coarse grained force fields.

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During the workshop, we will present a generic top-down strategy, based on an extended corresponding states framework, to build effective force fields for some coarse grained molecular models.
As an example the proposed strategy will be applied to the Mie-Chain model. It will be shown that such an approach, combined with classical molecular simulations, allows to provide a very good estimate of thermophysical (equilibrium, interfacial and transport) properties of some fluids typical of the oil and gas industry.
In addition, it will be shown how such an approach can be combined with modern molecular thermodynamics to yield thermophysical properties without molecular simulations.