

# 数学与系统科学研究院

## 计算数学所学术报告

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报告题目:

**Liquid-Vapor Phase Transition: Thermomechanical Theory, Entropy Stable Numerical Formulation, and Boiling Simulation**

邀请人: 唐贻发 研究员

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报告地点: 数学院南楼七层 702  
会议室

# **Abstract:**

Boiling flows are widely used as an energy transfer mechanism in practice. However, due to its disparity of spatiotemporal scales and elusive nature of many sub-processes, a complete theory of boiling is still lacking. Phase-field type multiphase flow models are considered well-suited for describing liquid-vapor phase transitions. However, the current study on these models mainly focuses on bubble dynamics and free surface problems. The full capability of phase-field type multiphase models has not been fully realized by the multiphase flow community.

In this work, we first systematically derive a new modeling framework for multiphase and multicomponent flows, using the celebrated microforce theory developed by Gurtin [2]. One very desirable feature of this framework is that once the explicit form of the thermodynamic potential is given, the model is closed and intrinsically thermodynamically consistent. We will show that the thermomechanical theory derived by Dunn and Serrin [1] is a special case in this framework by choosing an appropriate thermodynamic potential function.

A new fully discrete scheme is constructed to solve the aforementioned thermomechanical theory, i.e., the Navier-Stokes-Korteweg equations. In particular, the spatial discretization is designed based on the notion of functional entropy variables. A new time integration scheme is constructed based on a pair of special quadrature rules. The resulting fully discrete scheme is provably entropy dissipative and second-order accurate in time. Isogeometric analysis [3] is invoked to implement the numerical scheme.

The pool boiling problem is numerically investigated by making proper assumptions on transport parameters and boundary conditions. Compared with traditional multiphase solvers, the dependency on empirical data is significantly reduced for boiling simulations. It will be demonstrated that this modeling approach provides a unified predictive tool for both nucleate and film boiling. Both two and three-dimensional simulation results will be provided and discussed

## References

- [1] J.E. Dunn and J. Serrin. On the thermomechanics of interstitial working. *Archive for Rational Mechanics and Analysis*, 88:95–133, 1985.
- [2] M.E. Gurtin. Generalized Ginzburg-Landau and Cahn-Hilliard equations based on a micro-force balance. *Physica D: Nonlinear Phenomena*, 92:178–192, 1996.
- [3] T.J.R. Hughes, J.A. Cottrell, and Y. Bazilevs. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry, and mesh refinement. *Computer Methods in Applied Mechanics and Engineering*, 194:4135–4195, 2005.

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