



The Hong Kong University of Science and Technology

Department of Mathematics

PhD THESIS EXAMINATION

**Towards Physical AI: Physical Simulation,
Generative Modeling, and Embodied Interaction**

By

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ABSTRACT

Physical Artificial Intelligence (Physical AI) seamlessly integrates artificial intelligence with physical systems to enable intelligent perception, inference, and real-world interaction. Despite its promise, Physical AI faces significant hurdles in the construction of simulation infrastructure, generative modeling brain, and embodied interaction systems. This thesis aims to make contributions across three key tasks above: physical simulation with remeshing, generative field-to-field probabilistic modeling, and embodied contact-rich manipulation, thereby substantially advancing the field of Physical AI.

In the first part, we explore the simulation infrastructure and present OmniRemesh, a physical simulation remeshing framework in the context of crystal plasticity, which supports stable forward simulation capable of capturing local details, as well as inverse constitutive-parameter identification. OmniRemesh dynamically refines the mesh topology near grain boundaries and high-plastic-activity zones based on a designed size field, followed by variable transfer and equilibrium projection. To support inverse parameter identification despite discrete topology changes, OmniRemesh adopts frozen remeshing branches within trust regions, allowing constitutive parameters to be identified using automatic differentiation. Some numerical results verify the effectiveness of the framework.

In the second part, we study the generative modeling brain, and AlloyVAE is proposed to model the inherently probabilistic field-to-field relationships of alloys that arise when microstructural descriptors do not uniquely determine mechanical fields. Using a conditional variational autoencoder with learned smoothing operators and a self-consistency mechanism, it learns the conditional distribution of residual-stress fields from composition and short-range-order inputs, rather than collapsing them into a single deterministic prediction. Beyond forward generation of multiple physically admissible realizations under the same condition, the framework also supports gradient-based inverse design and extends naturally to coupled mappings involving eigenstrain.

In the final part, we focus on the embodied manipulation and propose Tac2Real, a lightweight visuotactile simulation framework designed to enable efficient online reinforcement learning (RL) training and sim-to-real transfer. Tac2Real integrates the Preconditioned Nonlinear Conjugate Gradient Incremental Potential Contact (PNCG-IPC) method with a multi-node, multi-GPU high-throughput parallel simulation architecture, which can generate marker displacement fields at interactive rates. Meanwhile, we propose a systematic approach, TacAlign, to narrow both structured and stochastic sources of domain gap, ensuring a reliable zero-shot sim-to-real transfer. We further evaluate Tac2Real on the contact-rich peg insertion task. The zero-shot transfer results achieve a high success rate in the real-world scenario, verifying the effectiveness and robustness of our framework.

Together, these works advance Physical AI through a unified progression from physical simulation, generative probabilistic modeling, to embodied manipulation. They provide a foundation for intelligent systems that can facilitate modeling, inference, and iteration in the physical world.

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Thesis Examination Committee:

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(Open to all faculty and students)

The student's thesis is now being displayed on the reception counter in the General Administration Office (Room 3461).