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(G) (POS-62) SymPhas: A general purpose C++ software for phase-field simulations

Tuesday 28 May 2024 18:01 (2 minutes)

We present an open-source API and software package called SymPhas for defining and simulating phase-field models, supporting up to three dimensions and an arbitrary number of fields. SymPhas is the first of its kind to offer complete flexibility in user specification of phase-field models from the phase-field dynamical or free energy equations, allowing the study of a wide range of models with the same software platform. This is accomplished by implementing a novel symbolic algebra library with a rich feature set that supports user-defined mathematical expressions with minimal constraint on expression format or grammar. The symbolic algebra library uses C++ template meta-programming, meaning that all expressions are represented as a C++ type. Consequently, symbolic expressions are "static" and formulated at compile-time, including all rules and simplifications that are applied. This approach dramatically minimizes application runtime, particularly for complex models since branching is entirely eliminated from the symbolic evaluation step. Performance is also augmented via parallelization with OpenMP and the C++ standard library. SymPhas has been used to simulate a number of well-known phase-field models, most of which are available as examples [1], as well as generating large-scale training and test data for a machine learning algorithm [2].

1. Silber, S. A. & Karttunen, M. SymPhas —General Purpose Software for Phase-Field, Phase-Field Crystal, and Reaction-Diffusion Simulations. *Adv. Theory Simul.* **5**, 2100351 (2021).
2. Kiyani, E., Silber, S., Kooshkbaghi, M. & Karttunen, M. Machine-learning-based data-driven discovery of nonlinear phase-field dynamics. *Physical Review E* **106**, 65303 (2022).

Keyword-1

phase-field

Keyword-2

symbolic algebra

Keyword-3

high performance

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