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Propositions

accompanying the dissertation

Reliable and Data-Efficient Machine Learning for Tractable Multiscale Material Simulations

by

Joep STORM

- 1. Adaptively updating a surrogate during a simulation rests on the assumption that it cannot be trusted outside its training distribution. The case for this approach shrinks as physics-embedded extrapolation improves.
- 2. Graph neural networks are elegant but not simple, and simplicity is more important.
- 3. The foundations of surrogate-based multiscale simulation are sound. The problems worth solving next will surface through application in industry, not within academia alone.
- 4. Thermodynamic consistency in surrogate models can be beneficial, but is neither sufficient nor necessary, and can give a false sense of assurance.
- 5. The time spent accelerating code is proportional to the researcher's unwillingness to wait for it.
- 6. A conference should be judged by the collaborations it starts, not the talks it hosts, and by that measure most conferences fall short.
- 7. Implementing promising methods in in-house software, rather than maintaining them in an open-source library, is faster in the short term but wastes time overall.
- 8. Attention is our most important resource, and guarding it is increasingly necessary. In some sense, Attention Is All We Have.
- 9. If progress in general-purpose AI sustains its current rate, it will likely supersede human-led research within ten years. Society is dangerously unprepared for this scenario.

■ *This proposition pertains to the dissertation.*

These propositions are regarded as opposable and defensible, and have been approved as such by the promotor dr. ir. F. P. van der Meer and co-promotor dr. I. B. C. M. Rocha.