Propositions

accompanying the thesis

Aggregate, Assemble, Automate

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1. Most of the tools and code in molecular dynamics are limited to processing linear, unmodified, polymers — such as proteins and DNA — even though everyone knows both nature and the field are more complex.

   Chapter 2

2. Algorithms that are developed for stochastic processes do not necessarily work for other concepts, even those that can also be described as graphs.

   Chapter 3

3. When writing scientific software, special care should be taken to avoid implicit assumptions, lest your program is suddenly capable of solving only a single problem.

   Chapters 2 and 3

4. Development of new software and methods for science is science: based on the problem description assumptions and hypotheses are formulated, which are challenged by new implementations and test cases.
5. “Because without users, your program is pointless, and all the development work you’ve done over decades is pointless.”

   L.B. Torvalds

   This means making just a proof-of-concept implementation of a new algorithm or tool is a waste of time if this implementation is not made easily accessible to the community.
6. Picking appropriate colours for data visualisation takes thought. Luckily, many smart people have already thought about this.
7. You never have to teach anyone to make backups — they teach themselves.

   K.R. Loopstra

8. Sticking your head in the sand won’t make problems go away. Talking to your supervisor(s) might.
9. Higher education should be free for all, since it benefits all of society to have lawyers write and debate law; artists make art in all its forms and shapes; and scientists make today’s impossibles tomorrows commonplace.
10. When playing dice games a lower variance might be preferable over a higher average.