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Aggregate, automate, assemble

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Finally, at the risk of sounding pedantic, some advice to new (PhD) students: firstly, read the Gromacs user list and the Martini forum, if only to learn from other people's mistakes. Secondly, join for coffee breaks, lunch, and other social events. Knowing your colleagues more informally makes it easier to ask them questions. Thirdly, if you end up writing software, read something on good software development practices, possibly focussed on science. That way you don't have to reinvent the wheel several times per week.