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A Communication Module for FMSolvr

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In the process of modularizing the molecular dynamics simulation library FMSolvr of JSC, we do not only want to improve our numerical methods but also take a look at communication and whether we can achieve an improvement on that front. We conducted a systematic literature review to see what has already been done in this field and picked out two promising communication schemes for further analysis: Shift communication as by Plimpton (1993) and a processor team-based approach by Driscoll, Georganas and Koanantakool (2013). Now, we are focused on finding a formal way of modelling these approaches in the hopes that it will help us with finding a formula for the trade-off point between one and the other method. The calculation of this trade-off point will be part of the communication module, which based on the result decides which communication method is best applied for the given input values of the simulation.

JLESC topic

communication in HPC

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