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Discontinuous Galerkin solver for continuous chromatography

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Column chromatography is a workhorse unit operation for purification of proteins and pharmaceuticals. Most column chromatography unit operations are run in batch-mode although continuous chromatography has the potential to increase productivity and reduce the solvent consumption. Operating continuous chromatography requires having multiple columns in series and/or parallel. The operation is thus significantly more complex compared to batch chromatography, but modelling can aid the operation of them. However, modelling of continuous chromatography also becomes more complex compared to batch operation for the following reasons: 1) When having columns in series, the system will consist of coupled partial differential equations that must be solved simultaneously. 2) The system can never reach steady state because of the nature of the separation process but can reach a cyclic steady state. For some continuous chromatography operations, it is required to simulate far into the future to reach the cyclic steady state, leading to long simulation times. 3) Continuous chromatography has switches of flowrates (events) leading to periodic discontinuities.
These factors lead to long simulation times. Thus, optimization of operation becomes very time consuming. Therefore, fast solvers are needed to enable real-time optimizations which is required for developing digital twins.
The most widespread simulation software for continuous chromatography is the open-source software called CADET which uses a finite volume method to solve the underlying PDEs. So far, only Kristian Meyer has developed and implemented a Discontinuous Galerkin spectral element method for solving the underlying PDEs for batch chromatography [1]. To develop a faster solver, the work of Kristian Meyer is extended to multiple columns and is implemented in Julia. The performance of the Discontinuous Galerkin solver is tested by comparing against CADET. The implementation of the Discontinuous Galerkin solver has the potential to decrease the simulation times enough to enable real-time optimizations.

[1]: Meyer, K., Leweke, S., von Lieres, E., Huusom, J. K., 38; Abildskov, J. (2020). ChromaTech: A discontinuous Galerkin spectral element simulator for preparative liquid chromatography. Computers and Chemical Engineering, 141, 107012. https://doi.org/10.1016/j.compchemeng.2020.107012

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