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Review on the Doctoral thesis “Extension of smoothed particle hydrodynamics based on Poisson brackets” by Ondřej Kincl

Topic of the thesis is an extension of the *Smooth Particle Hydrodynamics (SPH)* method to more general classes of applications. In particular, Kincl considers Hamiltonian systems given by Poisson brackets.

The thesis is handed in as a short summary of the work pursued during the doctoral studies. Details are given in three papers that have all appeared in good journals:

- J1) **Ondřej Kincl** and Michal Pavelka. Globally time-reversible fluid simulations with smoothed particle hydrodynamics. *Computer Physics Communications*, 284:108593, 2023.
- J2) **Ondřej Kincl**, Ilya Peshkov, Michal Pavelka, and Vaclav Klika. Unified description of fluids and solids in smoothed particle hydrodynamics. *Applied Mathematics and Computation*, 439:127579, 2023.
- J3) **Ondřej Kincl**, David Schmoranzer, and Michal Pavelka. Simulation of superfluid fountain effect using smoothed particle hydrodynamics. *Physics of Fluids*, 35(4), 2023.

Second and third paper more or less reflect the work described in sections 2 and 3, whereas parts of the first paper are found in Section 1. The work is in the field of scientific computing. Complex models are discretized using modern and efficient methods.



Structure of the thesis

The first section is devoted to a brief introduction to SPH and its application to isentropic compressible fluids. This also includes a little survey on convergence results for SPH. In what follows, time discretization methods with symplectic integrators are introduced. Finally, approaches to include viscous effects are discussed such that Navier-Stokes models are covered. The special difficulty lies in avoiding second derivatives of the smoothing kernels. The first section concludes with a numerical example modeling a dam break scenario.

In the second chapter, which includes substantial new results, Kincl extends the SPH method to *symmetric hyperbolic thermodynamically compatible (SHTC) models*. This modeling framework allows for a seamless transition between different fluid- and solid models. Besides basic modeling, Kincl discusses similarities to the Navier-Stokes model. For discretization with SPH, renormalization matrices are introduced for higher order conservation. Two numerical examples demonstrate the potential for one solid and one fluid problem.

The third and last section is dealing with a challenging application problem, the modeling of superfluid Helium. Kincl starts with describing a two-fluid model. The special difficulty of this model is that it cannot be written such as typical multiphase systems that consist of two separate laws for conservation of mass. Instead, the model must more be seen as a material with two interacting velocities. Hence, besides a description of the SPH discretization, special attention is given to the proper formulation of the specific energy. Finally, two numerical examples are demonstrated, among them, an interesting test case demonstrating the fountain effect for superfluids.

Notes on the journal articles

J1) The first paper appeared in *Computer Physics Communications* and describes an SPH realization that gives a fully time-reversible implementation. To achieve time-reversibility, some care has to be taken with the initial condition and, more specifically, numerical arithmetics must be realized such that calculations are associative. This is finally presented with the dam break problem that, at a fixed point in time is run backward to initial time and initial condition.

J2) This paper, published in *Applied Mathematics and Computations*, covers the second chapter of this thesis. In addition to what has been described above, numerical 3d examples are shown and the paper includes detailed discussion of the results.



J3) Published in *Physics of Fluids*, the third paper corresponds to section 3 and covers the superfluid Helium problem. It, in particular, includes a comprehensive description of the numerical test case.

Assessment of the work

In his thesis, Kincl works with physically sophisticated models and discusses appropriate numerical methods. The overall topic is very complex. The approaches chosen are appropriate to the models and the description of the work, especially in the journal articles, is of the highest level. The work meets the requirements of a doctoral thesis in every respect in terms of complexity, scope, implementation and mathematical presentation.

There remain a few points that could be better highlighted, especially in the short summary of the work, and which cannot be completely clarified even with the help of the three articles.

- 1) The three papers were each written in a team with one, two or three other co-authors. It is therefore not easily possible to precisely identify Kincl's contribution to the work. This could have been clearly indicated as part of the thesis.
- 2) The situation is similar with the presentation of the theoretical results in the work. After the brief description in the introduction, I assume that these theoretical results in Section 1.3 are taken from the literature. Precise information would be desirable here.
- 3) The topic of the work is the application and further development of SPH for various complex models. As part of the summary, it would be interesting to learn more about the relationship to alternative formulations and discretizations. Likewise, the numerical complexity of the methodology and how it relates to alternative approaches, is not completely clear.
- 4) The effect of using fixed point arithmetics to reach reversibility is fascinating. Without special treatment of the summations, the results change drastically. Intuitively, I would expect that this effect should, on the other hand, lead to stability problems and rounding errors of equal impact. A closer analysis would be highly interesting.

I recommend acceptance of this very interesting thesis without restrictions.

With best regards,

Prof. Dr. Thomas Richter