Received: 8 June 2020 | Accepted: 24 November 2020

DOI: 10.1002/pamm.202000044

Integral jump conditions for singular problems – applied to Debye-layer phenomena

Philipp G. Marthaler[1,*] and **Andreas G. Class**[1,**]

[1] Institute for Thermal Energy Technology and Safety (ITES), Karlsruhe Institute of Technology (KIT), Herrmann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

In numerical simulations boundary layers can be treated as jump conditions inheriting detailed physical effects that emerge inside the thin layer. The presented approach, first applied by Class et al. [3], is used to determine such jump conditions in integral form. It is applied to an electro-hydrodynamic problem with a Debye-layer in direct vicinity to a charged solid wall.

1 An integral method for boundary layers

A wide range of fluid-dynamic boundary layer problems have been the subject of ongoing investigations, such as boundary layers near a solid surface as well as thermal, gasdynamic or electro-hydrodynamic boundary layers. These problems are generally described as sets of nonlinear differential equations whose highest derivative is multiplied by a perturbation parameter δ. Their solutions change rapidly within the small layer whose thickness becomes zero for $\delta \to 0$. [2]

The purpose of the presented method is to make a numerical treatment of boundary layer problems possible. The computational domain is therefore decomposed into two smaller domains, separated by the boundary layer. Then, both sub-domains can be coupled using a jump condition for the normal flux through the discontinuity surface. For each physical parameter (and equation) of interest we can find one jump condition which replaces the detailed treatment of all effects inside the layer.

The objective is to derive time-dependent jump conditions for the normal flux emerging at boundary layers of arbitrary shape. Tensor notation and asymptotics have first been applied by Class et al. for the description of flames. [3] Here, the method is applied to electro-hydrodynamic (EHD) double layers emerging at the interface between charged solids and fluid electrolyte. For each physical parameter $\phi\left(x^j, t\right)$ we can formulate a transport equation of the generic contravariant form

$$\partial_t \left(\sqrt{g}\,\phi\right) + \partial_{x^j}\left(\sqrt{g}\,J^j\left(\phi\right)\right) = \sqrt{g}\,S\left(\phi\right), \tag{1}$$

including the generic fluxes $J^j\left(\phi\right)$ and the source term $S\left(\phi\right)$. Furthermore, we assume that the surface can at each point be described by the contravariant metric $g^{ij}\left(x^j, t\right)$. We define x^1 as the normal coordinate so that the metric can be specified by $g^{11} = 1$ and $g^{i\alpha} = 0$[1]. From the metric we find the volume element $\sqrt{g}\left(x^j, t\right) = {}^1/_{\det\left(g^{ij}\right)}$ which appears in the generic transport equation (1). We can now define two models, the detailed and the hydrodynamic model. In the detailed model all parameters, denoted by capital letters Φ, are continuous and all physical effects are considered. The hydrodynamic model consists of the same equations but is lacking at least one term, usually a source term. The missing terms are then taken into account in form of the jump conditions of the parameters ϕ at the discontinuity surface.

In order to find the desired jump conditions that we define as $\left[J^1\left(\phi\right)\right] = J^1\left(\Phi\right) - J^1\left(\phi\right)$ we consider the difference between both model's transport equations integrated over the normal derivative

$$\int_{x^1_\mathrm{l}}^{x^1_\mathrm{r}} \partial_t\left(\sqrt{g}\,\left(\Phi-\phi\right)\right)\mathrm{d}x^1 + \sqrt{g}^*\left[J^1\left(\phi\right)\right] + \int_{x^1_\mathrm{l}}^{x^1_\mathrm{r}} \partial_{x^\alpha}\left(\sqrt{g}\,\left(J^\alpha\left(\Phi\right) - J^\alpha\left(\phi\right)\right)\right)\mathrm{d}x^1 = \int_{x^1_\mathrm{l}}^{x^1_\mathrm{r}} \sqrt{g}\,\left(S\left(\Phi\right) - S\left(\phi\right)\right)\mathrm{d}x^1. \tag{2}$$

The integration is performed from a position x^1_l sufficiently far "left" from the discontinuity surface (which we define at $x^1 = x^{1*}$) to a position sufficiently far "right" that the differences between both models vanish. Thus, if $x^1_\mathrm{l} \to -\infty$ and $x^1_\mathrm{r} \to \infty$ the integrals are still determined. The following steps are similar to classical boundary layer theory [2, 5]. The normal coordinate is stretched by the perturbation so that we find the stretched coordinate $X = {}^{x^1}/_{\delta}$. Both models' parameters are expanded in terms of the Taylor series and the solutions for the leading order(s) are determined. Finally, these solutions are employed into equation (2) written in terms of the stretched coordinate

$$\sqrt{g}^*\left[J^1\left(\phi\right)\right] = \int_{-\infty}^{\infty}\left(\sqrt{g}^*\left(S\left(\Phi\right) - S\left(\phi\right)\right) - \partial_t\left(\sqrt{g}^*\left(\Phi-\phi\right)\right) - \partial_{x^\alpha}\left(\sqrt{g}^*\left(J^\alpha\left(\Phi\right) - J^\alpha\left(\phi\right)\right)\right)\right)\mathrm{d}X \tag{3}$$

which results in the jump of the normal flux.

* Corresponding author: e-mail philipp.marthaler@kit.edu, phone +49 721 608 25781

** e-mail andreas.class@kit.edu

[1] The greek indices describe the tangential directions and can be 2 or 3 while the latin indices can be 1, 2 or 3.

2 Application to streaming-potential phenomena

We apply the described method to a class of stationary streaming-potential phenomena, which was discussed before by [4,6,7]. The dimensionless thickness of the Debye-layer in vicinity to a charged surface is supposed to be small and therefore used as perturbation parameter δ. We use the same reference dimensions as described in the flow-driven problem in [7], with the Péclet-number $\mathrm{Pe} \sim O\left(\delta^{-2}\right)$, the Hartmann number $\lambda \sim O\left(1\right)$ and the Schmidt number $\mathrm{Sc} \ll 1$ sufficiently small so that the transient and convective terms of the momentum equation can be neglected. The flow problem is defined by the momentum and incompressible continuity equations while the Poisson-Nernst-Planck system describes the distribution of charges and electric potential. The coupling emerges in form of the Maxwell stress tensor in the momentum equations and the convective term in the Nernst-Planck equations.

Now, we define the EHD model as the detailed model. In Poisson's equation it includes the charge density which is neglected in the hydrodynamic model with jumping parameters. The jump condition for the electric potential ψ can be found easily using the Gouy-Chapman solution of the 1D-problem at leading order [7]. With the charge density $S\left(\Psi\right) = -\sinh\left(\Psi\right) + O\left(\delta\right)$ and $S\left(\psi\right) = -\sinh\zeta$ for $X \in [0, X^*]$ and $S\left(\psi\right) = 0$ for $X \in [X^*, \infty)$ we can adapt equation (3) to find

$$\left[J^1\left(\psi\right)\right] = \int_0^\infty S\left(\Psi\right) - S\left(\psi\right) \mathrm{d}X = \left(-2\sinh{}^{\zeta}\!/\!{}_2 + X^* \sinh\zeta\right) + O\left(\delta\right). \tag{4}$$

In case of a solid wall right next to the discontinuity surface the lower limit for integration is the wall, defined as $x^1_{\mathrm{wall}} = 0$. The zeta-potential was utilized as boundary condition $\Psi\left(X = 0\right) = \zeta$. The position X^* at which the outer term jumps can be chosen such that the integrals can be solved easily. For the charge density we can derive a similar jump condition

$$\begin{aligned} \left[J^1\left(q\right)\right] &= -{}^1\!/\!{}_{\sqrt{g^*_{(0)}}}\,\partial_{x^\alpha}\left(\sqrt{g^*_{(0)}}\left(J^\alpha\left(Q\right) - J^\alpha\left(q\right)\right)\right)\mathrm{d}X \\ &= \mathrm{Pe}_{(-2)} D \int_0^\infty X\left(Q_{(0)} - q_{(0)}\right)\mathrm{d}X = \mathrm{Pe}_{(-2)} D\left(\zeta + \sinh\zeta\left({}^1\!/\!{}_2 (X^*)^2 + X^*\right)\right) + O(\delta). \end{aligned} \tag{5}$$

The sum of the (convective) tangential fluxes $J^\alpha\left(Q\right)$ has been transformed using the continuity equation to obtain a result depending on the normal velocity $V^1_{(2)} = {}^D\!/\!{}_2 X^2$. This procedure as well as the choice of the parameter D is the same as in [7]. For the flow problem we obtain four jump conditions. For the pressure we obtain

$$\left[J^1\left(p\right)\right] = \delta\lambda_{(0)} g^{\alpha\beta}\partial_{x^\alpha}\varphi\left(2X^*\sinh{}^{\zeta}\!/\!{}_2 - \zeta\right) l_\beta + O(\delta^2). \tag{6}$$

The other results for the flow also contain the Smoluchowski slip velocity $v_{\mathrm{slip}} = \zeta\lambda_{(0)} g^{\alpha\beta}\partial_{x^\alpha}\varphi\, l_\beta$ which depends on the outer potential φ and the tangential vector l_β. They can be derived in a similar way from the continuity equation and the momentum equation in tangential direction.

3 Conclusion

The presented approach allows the numerical treatment of singular problems through the use of jump conditions. Thereby, the jump conditions inherit the detailed modelling of the phenomena responsible for the emergence of the double layer.
As an example we applied the method to a stationary EHD problem which has been discussed in literature by different authors. Our leading order solutions are in accordance with Yariv et al. [7]. The derived integral form of the jump conditions shall be applied for numerical simulations in the future. Furthermore, the stationary model will be extended to consider instationary effects. This makes only sense using a hybrid approach of asymptotic and numeric computations as the leading order solution has to be computed numerically as well.

Acknowledgements We acknowledge the Framatome Professional School for support.
Open access funding enabled and organized by Projekt DEAL.

References

[1] R. Aris, Vectors, Tensors, and the Basic Equations of Fluid Mechanics (Dover Publ., New York, 1989).
[2] C. M. Bender, S. A. Orszag, Advanced Mathemetical Methods for Scientists and Engineers I (Springer, New York, 1999)
[3] A. G. Class, B. J. Matkowsky and A. Y. Klimenko, J.F.M. **491**, pp. 11–49 (2003).
[4] R. G. Cox, J.F.M. **168**, pp. 169–194 (1986).
[5] E. J. Hinch, Perturbation Methods (Cambridge Univ. Press, Cambridge, 2002).
[6] M. Smoluchowski, Handbuch der Elektrizität und des Magnetismus II (Barth, Leipzig, 1921)
[7] E. Yariv, O. Schnitzer and I. Frankel, J.F.M. **685**, pp. 306–334 (2011).

