AN INVERSE FORMULATION FOR SOLUTION OF FREE–BOUNDARY PROBLEMS IN FLUID MECHANICS

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ABSTRACT

This investigation is motivated by the problem of optimization of interfacial thermo–fluid phenomena occurring in advanced welding processes. In the first part of the presentation we consider a 3D multiphysics problem involving complex fluid flow combined with heat transfer and interfacial (Marangoni) effects in a weld pool with free boundaries [1,2]. We demonstrate how the problem of finding a steady–state solution in such a free–boundary problem can be reformulated as an inverse (optimization) problem in which a suitable cost functional is minimized with respect to the geometry of the interfaces and/or interfacial values of the control parameters, and subject to PDE constraints. An advantage of this formulation is that it allows for a thermodynamically consistent treatment of the interface and contact–line conditions. In particular, it makes it possible to introduce closure models for unresolved thermodynamic parameters defined at the microscopic level in a natural way. We describe an efficient iterative solution method for this problem which uses shape differentiation, adjoint equations, and Sobolev inner products to determine consistent gradients of the cost functional. We show evidence that the proposed method captures the correct flow patterns in the weld pool for the surface tension either increasing or decreasing with the temperature. In the second part of the presentation we discuss an extension of this inverse formulation which accounts for the mass transfer into the weld pool. As a part of this investigation we derive equations characterizing an "effective" free–surface obtained by averaging the time–dependent free–boundary equations in the volume–of–fluid (VoF) formulation. We highlight the role of the closure models required to represent the terms which, in analogy with the Reynolds stresses in classical turbulence models, arise from fluctuations of the free boundaries. We argue that such effective free boundaries can also be conveniently computed via an inverse (optimization) formulation in which a suitable cost functional is minimized with respect to the position of the effective interface. A key advantage of such an approach is that the effective free boundary is stationary which considerably simplifies framing inverse problems in which optimal control parameters are determined. Finally, we discuss examples of inverse formulations in which optimal inputs to the system can be determined.

REFERENCES

[1] O. Volkov and B. Protas, An inverse model for a free–boundary problem with a contact line: steady case, *Journal of Computational Physics* **228**, pp. 4893–4910 (2009).

[2] O. Volkov, B. Protas, W. Liao and D. Glander, Adjoint–Based Optimization of Thermo–Fluid Phenomena in Welding Processes", *Journal of Engineering Mathematics*, **65**, pp. 201–220 (2009).