Vaughan R. Voller, University of Minnesota, volle001@umn.edu
Free and Moving Boundary Problem Notes

Definition of a Moving Boundary Problem

In many problems in science and engineering the location of one or more of the domain boundaries is not known a-priori. Solution of these problems requires the tracking of a moving boundary (e.g., the liquid-solid front during a melting of freezing process, see Fig. 1.1a) or the determination of the location of a free boundary (e.g., the water table in a ground water flow problem). In order to achieve the tracking or location of the boundary the problem specification must include an additional boundary condition on the free or moving boundary; typically a Dirichlet (a specified flux) and a Neumann (a specified value) condition are applied.

The Essential Difficulty

There are only a limited number of closed form solutions for moving boundary problems and in most problems of engineering or scientific interest numerical solutions are required. Numerical approaches use a discretization of the problem domain consisting of a grid of node points that define a mesh of elements, Fig. 1.2. The numerical solution is developed by appropriate representation of the governing equations over this grid. The result is in an algebraic system of equations in the nodal values of the dependent variables. In arriving at these equations, the preferred approach is to use an Eulerian grid of nodes that remain fixed in space throughout the calculation. In seeking numerical solutions of moving boundary problems, however, unless other actions are taken, the use of an Eulerian grid may not be possible. The essential difficulty is that discrete representations of conditions on the moving boundary will require information (e.g., the location of the boundary) not directly available from information stored at the fixed node points. Broadly, there are three ways of constructing discretizations for moving boundary problems that alleviate this difficulty.

1.Fixed Grid Methods

The first approach retains the use of a fixed space grid but extends the problem formulation to include an auxiliary variable that tracks the position of the moving boundary. Nodal values of the auxiliary variable, calculated on an Eulerian grid (fixed mesh), can then be used to reconstruct moving boundary information such as shape and position.

A basic fixed grid method is the so-called Volume of Fluid (VoF) method [1]. In this method, nodal value of a "liquid fraction" $0 \le g_P \le 1$ can be used to determine the amount of the volume, associated with node P, that is covered by the boundary—a value of $g_p = 0$ indicates that the boundary has not reach the volume around node p and a value of $g_p = 1$ indicates that the boundary has passed through the volume—see Fig. 1.3. The classical useVoF is the tracking of free surface flows, the term VoF, however, can be applied to any fixed grid method employing a continuity satisfying volume fraction field to track a moving boundary. In particular the definition includes fixed grid enthalpy methods [2-4] developed for moving boundary problems related to freezing and melting.

Alternative fixed grid methods include (i) Level set methods [5,6], where nodal values of an order parameter $-1 \le \phi \le 1$ provide a measure of the distance from a moving interface $\phi = 0$ and Phase field methods [7-12], where thermodynamic principals are used to arrive at a reaction-diffusion equation in terms of an auxiliary variable $-1 \le f(x) \le 1$. Level set calculations retain a sharp definition for the moving boundary interface, whereas, in a phase field method, the boundary is modeled as a diffusive interface. In the limit of a vanishing interface thickness, however, it can be theoretically shown, that the phase field model for a given moving boundary system approaches the required sharp interface model [7,8].

2. Deforming-Adaptive Mesh: The obvious, but not necessary the easiest means of tracking a moving boundary on a discrete description, is to use a Lagrangian discretization. This approach continuously deforms the numerical mesh ensuring that a line of node points is always located on the moving boundary. The classic application dates back to 1959 when Murray and Landis [13] solved one-dimensional melting and freezing problems with an expanding grid containing a fixed number of nodes. In multi-dimensional implementations operational problems can occur when the grid needs to undergo excessive distortion to conform to the moving boundary shape. Such problems can be controlled by adaptive updating that add or subtracts node points to maintain sound grid properties—see Fig. 1.4. A general description of the use of deforming meshes is found in Demirdžic and Petic [14], and examples of moving boundary applications in Lynch and O’Neill [15], Lynch [16], Beckett et al [17]. An example of an adaptive mesh that concentrates elements on the moving boundary but relaxes the condition for a line of node to coincide with the front is found in the simulation of dendritic growth presented by Provatas et al [11].

3. Hybrid: In addition to the application of fixed or deforming grid methods a hybrid that combine features of both Eulerian and Lagrangian can be used to track moving boundaries.

Once again the classic one-dimensional examples date back to the mid 1950's. Douglas and Gallie [18] analyzed a moving boundary by using combination of a fixed space grid with a variable time step. In the solution the time step is calculated so that the boundary moves from one node point to the next. In this way the moving boundary is constrained to always be located on a node. Crank [19] employed a local front tracking. With reference to Fig. 1.5, as the front s(t) moves through volume P its node point is replaced, in finite difference discretizations, by the node point located on the moving front.

In keeping with the one-dimensional Crank front tracking solution, multi-dimensional hybrid methods, use a fixed Eulerian background mesh for calculation of the main field variables and employ various interpolation techniques and interface conditions to continuously reconstruct a geometric description of the interface that cuts through the elements of the background mesh. Examples include an (i) update of the Crank local front tracking to two dimensional domains, discretized using both finite differences [20] and finite elements [21,22], and (ii) so-called "immersed" interface methods. The later method uses a fixed Eulerian grid to solve for the main dependent variables and employs a Lagrangian description based on a "string" of nodes to track the interface. In application to heat transfer problems, as described by Juric and Tryggvason [23], information is passed between the Eulerian grid and Lagrangian interface by distributing interface heat source to the grid and interpolating the grid temperatures to the interface nodes.

References

1. C.W. Hirt and B.D. Nichols, "Volume of Fluid (VOF) Method for the Dynamics of Free Boundaries," *J. Comp. Phys*., **39**, 201-225, 1981.

2. N.R. Eyres, D.R. Hartree, J. Ingham, R. Jackson, R.J. Sarjant, and S.M. Wagstaff, "The Calculation of Variable Heat Flow in Solids," *Phil. Trans. R. Soc*, **A240**, 1-57, 1946.

3. V.R. Voller and M.Cross, "Accurate Solutions of Moving Boundary Problem,s Using the Enthalpy Method," *Int. J. Heat Mass Transfer*, **24**, 545-556, 1981.

4 . J. Crank, *Free and Moving Boundary Problems*, Clarendon Press, Oxford, 1984.

5. J. A. Sethian, *Level Set Methods and Fast Marching Methods*, Cambridge University Press, Cambridge, 1999.

6. S. Chen, B. Merriman, S. Osher and P. Smereka, "A simple Level Set Method for Solving Stefan Problems," *J. Comp. Phys*., **135**, 8-29, 1997.

7. G. Caginalp, Stefan and Hele-Shaw Type Modules as Asymptotic Limits of the Phase-Field Equations," *Phys. Rev. A.,* **39**, 5887-5896, 1989

8. A. Karma and W.-J. Rappel, "Phase-field Method for Computationally Efficient Modeling of Solidification with Arbitrary Interface Kinetics, *Phys. Rev. E*, **53**, R3017-R3020, 1996.

9. A. Karma and W-J Rappel, "Quantitative Phase-Field Modeling of Dendritic Growth in Two and Three Dimensions," *Phys, Rev E*, **57**, 4323-4349, 1998.

10. C. Beckermann, H.-J. Diepers, I. Steinbach, A. Karma, and X. Tong, "Modeling of Melt Convection in Phase-Field Simulations of Solidification," *J. Comp. Phys*., **154**, 468-496, 1999.

11. N. Provatas, N. Goldenfeld and J. Dantzig, "Adaptive Mesh Refinement Computation of Solidification Microstructures using Dynamic Data Structures," *J. Comp Phys.*, **148**, 265-279, 1999.

12. W.J. Boettinger, J.A. Warren, C. Beckermann and A. Karma, "Phase-Field Simulations of Solidification," *Annu. Rev. Mater. Res.*, **32**, 163-194, 2002.

13. W.D. Murray and F. Landis, "Numerical and Machine Solutions of Transient Heat Conduction Problems Involving Melting or Freezing," *ASME J. Heat Transfer*, **81**, 106-112, 1959.

14. I Demirdžic and M. Peric, "Finite Volume Methods for Predicting of Fluid Flow in Arbitrarily Shaped Domains with Moving Boundaries," *Int. J. Num. Meth. Fluids*, **10**, 771-790, 1990.

15. D.R. Lynch and K. O'Neill, "Continuously Deforming Finite Elements for the Solution of Parabolic Problems with and without Phase Change," *Int. J. Num. Meth. Eng.*, **17**, 81-96, 1981.

16. D.R. Lynch, "Unified Approach to Simulation on Deforming Elements with Application to Phase Change Problems, *J. Comp. Phys.*, **47**, 387-411, 1982.

17. G. Beckett, J.A. Mackenzie and M.L. Robertson, "A Moving Mesh Finite Element Method for the Solution of Two-Dimensional Stefan Problems," *J. Comp. Phys.*, **168**, 500-518, 2001.

18. J. Douglas and T.M. Gallie, "On the Numerical integration of a Parabolic Differential Equation Subject to a Moving Boundary Condition," *Duke math. J.* , **22**, 557-571, 1955.

19. J. Crank, "Two Methods for the Numerical Solution of Moving Boundary Problems in Heat Flow, *Q. Jl. Mech. Appl. Math*. **10**, 220-231, 1957.

20. H.S. Udaykumar, R. Mittal and Wei Shyy, "Computation of Solid-Liquid Phase Fronts in the Sharp Interface Limit on Fixed Grids," *J. Comp. Phys.*, **153**, 535-574, 1999.

21. P. Zhao, J.C. Heinrich, "Front Tracking Finite Element Method for Dendritic Solidification," *J. Comp. Phys.*, **173**, 765-796, 2001.

22. P. Zhao, J.C. Heinrich and D.R. Poirier, "Fixed Mesh Front Tracking Methodologies for Finite Element Simulations," *Int. J. Num. Meth. Eng*., **61**, 928-948, 2004.

23. D. Juric and G. Tryggvason, "A Front Tracking Method for Dendritic Solidification," *J. Comp. Phys.*, ***123***, 127-148, 1996.

24. C. Elliott and J.R. Ockendon, *Weak and Variational Methods for Moving Boundary Problems*, Research Notes in Mathematics 59, Pitman, London, 1982.

25. D.A. Tarzia, Domingo, *A Bibliography on Moving-Free Boundary Problems for the Heat-Diffusion Equation. The Stefan Problem*. Inst. Mat. "Ulisse Dini". Univ. di Firenze. Firenze 1988.

26. V. Alexiades and A. D. Solomon, *Mathematical Modeling of Melting and Freezing Processes*, Taylor & Francis, 1992.

27. W. Shyy, H. S. Udaykumar, M. M. Rao and R. W. Smith, *Computational Fluid Dynamics With Moving Boundaries*, Taylor&Francis, Washinton 1995.

28. V.R. Voller, C.R. Swaminathan and B.G. Thomas, "Fixed Grid Techniques for Phase

Change Problems: A Review," *Int. J. Num. Meth. Eng.* **30**, 875-898, 1990.

29. V.R. Voller, "An Overview of Numerical Methods for Phase Change Problems," *Advances in Numerical Heat Transfer* **1**, 341-375, 1996.

30. H. Hu and S. A. Argyropoulos, "Mathematical Modeling of Solidification and Melting: A review," *Modelling Simul. Mater. Sci. Eng*. **4**, 371-396, 1996.

31. C. Beckermann and C.Y. Wang, "Multi-Phase/-Scale Modeling of Transport Phenomena in Alloy Solidification," *Annual Review Heat Transfer*, **6**, 115-198, 1995.

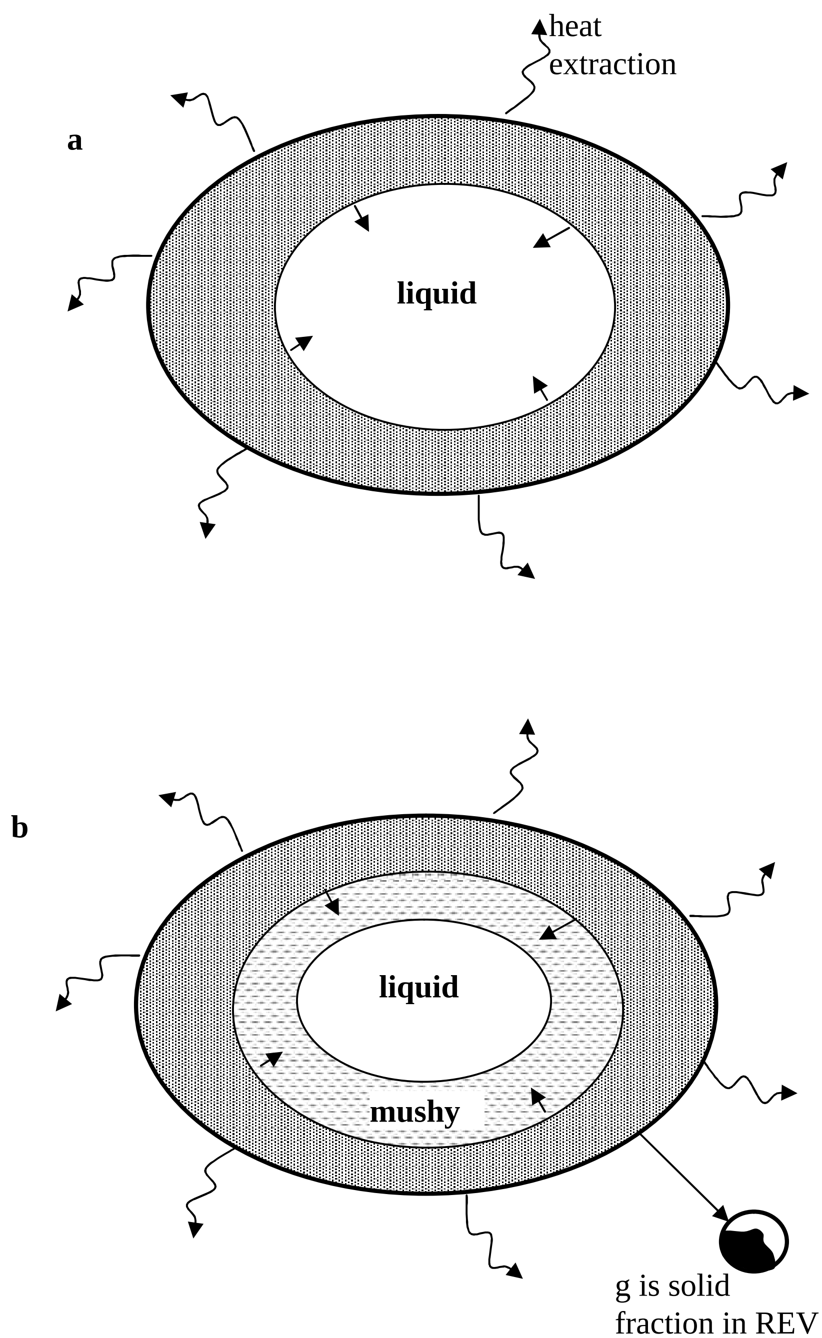


Figure 1.1: a. A moving boundary problem resulting from the solidification of a pure liquid. b. A phase change problem characterized by a solid+liquid mushy region.

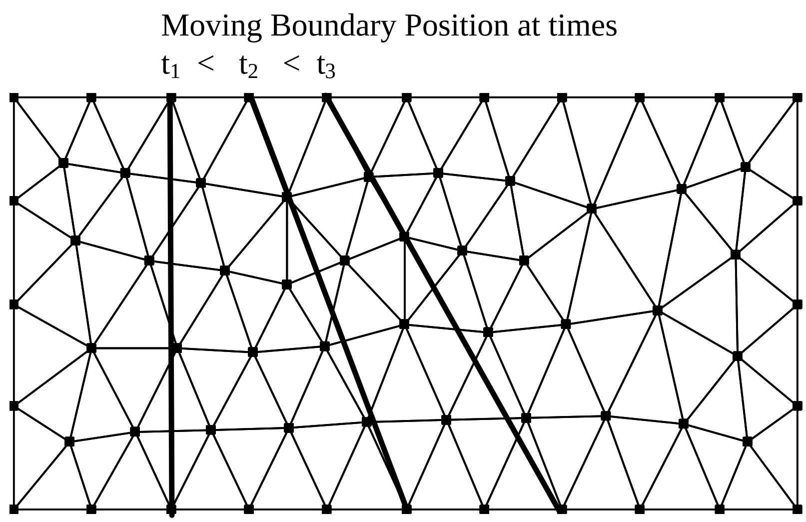
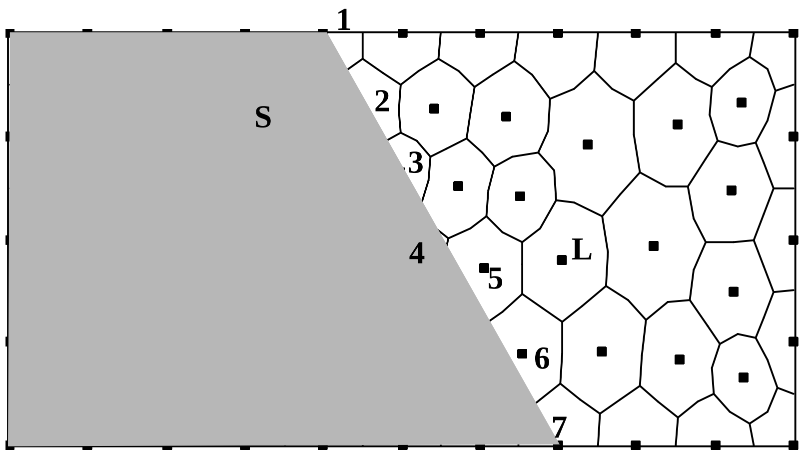


Figure 1.2: Position of a moving boundary relative to a fixed space grid. Note, by chance, only a limited number of node are on the boundary and the boundary does not coincide with element edges.



$g_S = 1,\ g_1 = 0.75,\ g_2 = 0.6,\ g_3 = 0.55,\ g_4 = 0.98,$
$g_5 = 0.25,\ g_6 = 0.3,\ g_7 = 0.3,\ g_L = 0$

Figure 1.3: Fixed Grid VOF approach for tracking the moving boundary. At a point in time the position of the boundary is located by specifying nodal "liquid" fractions that determine how mush of the associated nodal area is "covered" by the boundary.

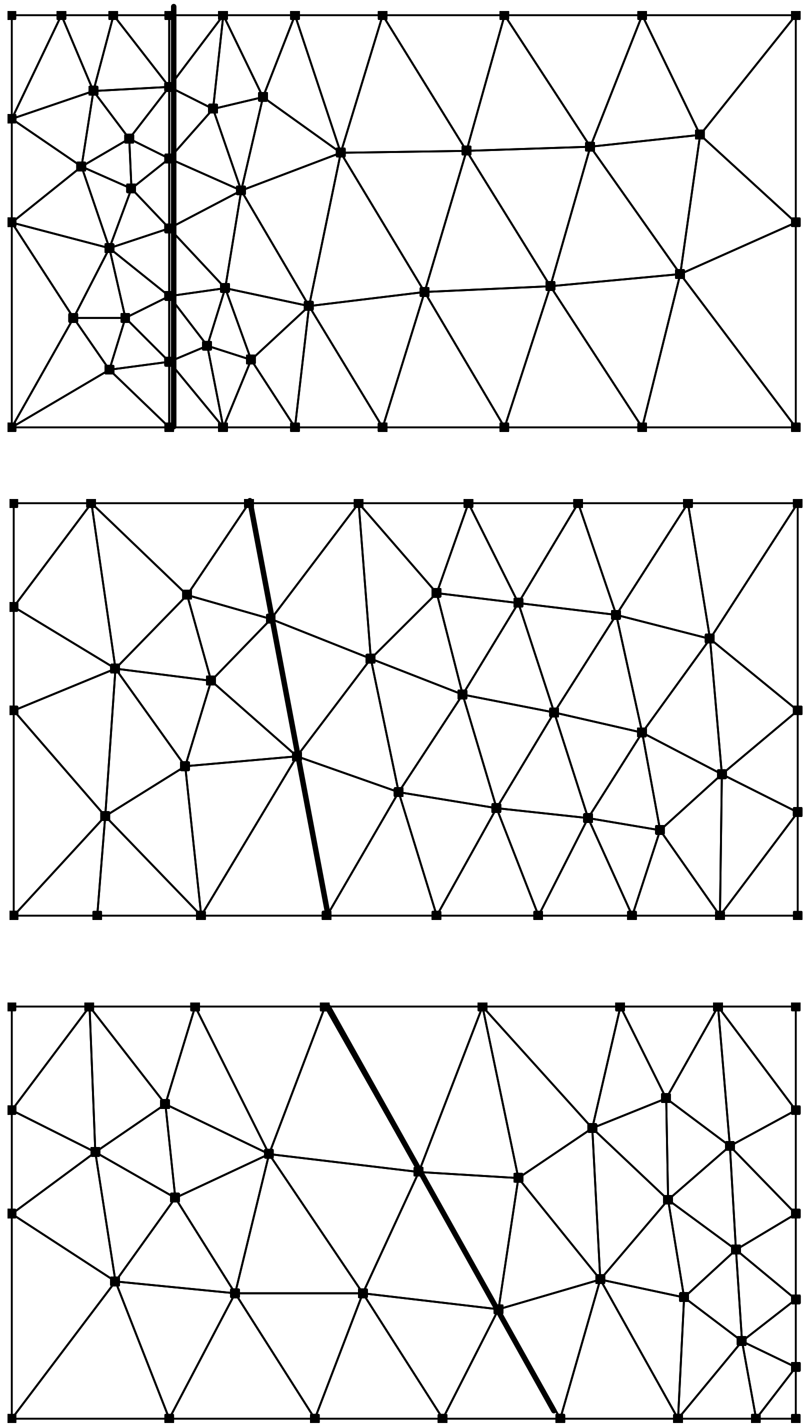


Figure 1.4 :Deforming Adaptive grid approach. The grid deforms and adapts at each time step to retain a sound grid properties and ensure that the moving boundary lies along element edges.

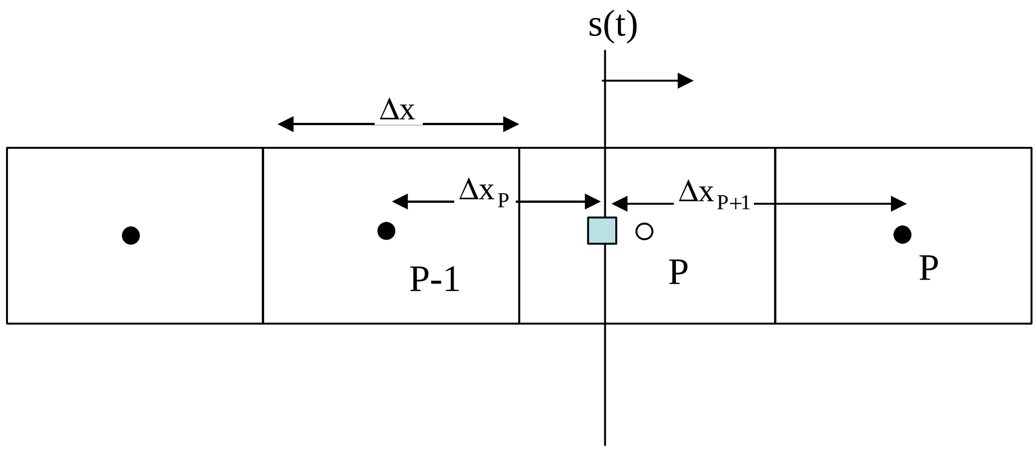


Figure 1.5 Illustration of one-dimensional local front tracking