Weak Formulation of Gradient Augmented Level set method to Stephan type problems

Lakshman Anumolu
CS838-Fall 2012
University of Wisconsin Madison

December 20, 2012

In this work, we present the application of weakly formulated gradient augmented level set method to Stephan type problem. Results for 3D test cases are presented and are rendered using mitsuba [Jakob, 2010].

1 Introduction

Problems associated with dendritic crystallization requires careful implementation of numerical methods. In the past few years various methods have been developed [F.Gibou et al., 2003; F.Gibou and R.Fedkiw, 2005] to track topologically complex, solid-liquid interface in crystal growth simulation.

In this work we employ gradient augmented level set method [Nave et al., 2010] to track interface. For maintaining signed distance function we implemented partial differential equation approach from [Anumolu and Trujillo, 2012] and also PhysBAM inbuilt fast marching method, but the results presented here use fast marching method. We discretize the heat equation on a Cartesian grid using implicit backward Euler method and for the nodes neighboring interface, the discretization is performed as proposed in [F.Gibou et al., 2003]. The jump in the first derivatives of the temperature is used to compute interface velocity and Gibbs-Thompson equation is used to compute temperature at the interface.

In the following sections, we first describe interface advection methods, followed by heat equation, which is followed by Stephan problem and finally we conclude with future work.

2 Level set Advection

Level set methods [Osher and Sethian, 1988] have gained considerable popularity in implicitly tracking interfaces. The main concern with these methods is the mass loss, in the recent years, there have been many methods which are proposed to improve the mass conservation property. Gradient augmented level set method also aim to solve this problem of mass conservation, where as this is acheived by tracking both the function and its gradient in a fully coupled fashion using cubic Hermite interpolating polynomials.

Generally the level set function (ϕ) is advected using the following equation

$$\frac{\partial \phi}{\partial t} + \mathbf{U} \cdot \nabla \phi = 0. \tag{1}$$

In gradient augmented level set method, Eq. (1) along with the transport equation for $\nabla\phi$ which is obtained by applying gradient on Eq. (1) is advected using semi-Lagrangian approach detailed in [Nave et al., 2010]. To briefly describe the semi-Lagrangian implementation, we identify the root of the characteristic by moving backward in time along the characteristic equation

$$\frac{d\mathbf{x}}{dt} = \mathbf{U}. \tag{2}$$

Once the root of the characteristic is identified, the level set and its gradient values at grid nodes can be updated by solving the following ordinary differential equations

$$\frac{d\phi}{dt} = 0, \tag{3}$$

and

$$\frac{d\psi}{dt} = -\nabla\mathbf{U} \cdot \nabla\psi, \tag{4}$$

where $\psi = \nabla\phi$. In this approach the root of the characteristic generally doesnot coincide with the grid node, hence it is required to compute the level set and its gradient values at locations other than grid nodes. Cubic Hermite interpolating polynomials are used to perform interpolation in this approach.

A 3D single vortex test case [Enright et al., 2002] is considered here, where a level set function defining the zero level set of sphere with radius 'r' given by

$$\phi(\mathbf{x}, t = 0) = \sqrt{(x - x_o)^2 + (y - y_o)^2 + (z - z_o)^2} - r, \tag{5}$$

is deformed under the influence of the velocity field given by

$$\begin{aligned} u(x, y, z) &= 2\sin^2(\pi x)\sin(2\pi y)\sin(2\pi z)\cos(\pi t/T), \\ v(x, y, z) &= -\sin(2\pi x)\sin^2(\pi y)\sin(2\pi z)\cos(\pi t/T), \\ w(x, y, z) &= -\sin(2\pi x)\sin(2\pi y)\sin^2(\pi z)\cos(\pi t/T). \end{aligned} \tag{6}$$

The sphere's center and radius are $(x_o, y_o, z_o) = (0.35, 0.35, 0.35)$ and $r = 0.15$ respectively. Figures 1a and 1b show the zero level set surface during initial and maximum deformation times ($T = 2.5$). For this test case, 5 reinitialization time steps are considered per each advection time steps.

3 Stephan problem

In the computational domain Ω, the governing equation for the Stephan problem is given by

$$\frac{\partial T}{\partial t} = \nu \Delta T \quad \mathbf{x} \in \Omega, \tag{7}$$

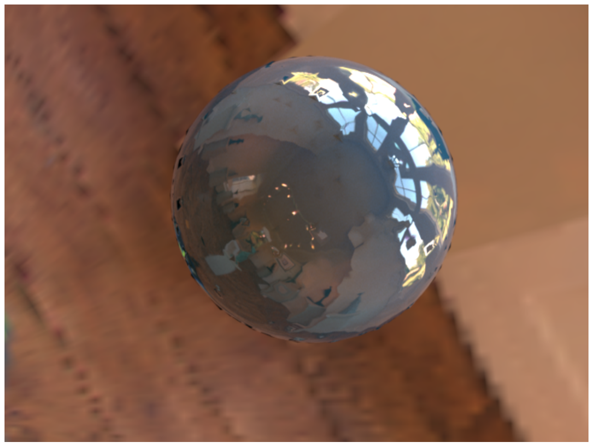
$$V_n = \nu\,[\nabla T] \cdot \mathbf{n}. \tag{8}$$

In this work, we considered Gibbs-Thompson relation [F.Gibou et al., 2003] at the interface, which is given by

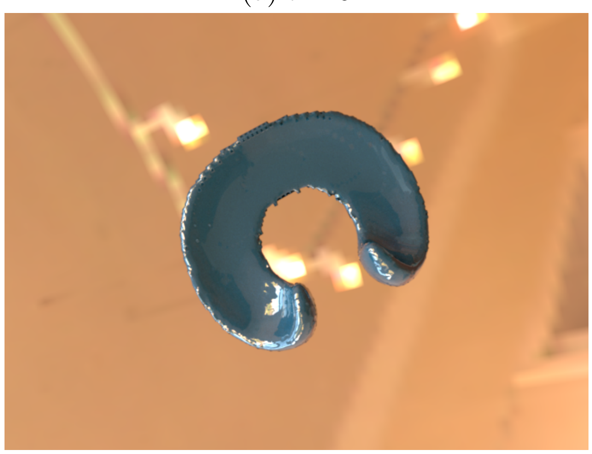
$$T_\Gamma = -\epsilon_c \kappa - \epsilon_v V_n, \tag{9}$$

where $\epsilon_c = \epsilon_v = .002$, κ is the curvature of the level zero level set.

The heat equation Eq. (7) is solved using implicit backward Euler method. While discretizing the heat equation, special care needs to be taken for the nodes adjacent to the interface, in this work we show the results from constant extrapolation, but the code written for this project can handle both constant and linear extrapolations. To obtain the interfacial velocity, which is given by the jump in the temperature gradient as given by Eq. (8), extrapolation of temperature fields is needed from one side of the interface to other side which can be either achieved by constant or linear extrapolations. In this



(a) $t = 0$



(b) $t = 2.5$

Figure 1: Sphere deforming in a single vortex flow field.

work we will show results obtained using constant extrapolation, but again the code has the capability to handle linear extrapolation. For more details regarding the underlying algorithms and more accurate discretizations and extrapolations, reader is adviced to refer [F.Gibou et al., 2003; F.Gibou and R.Fedkiw, 2005]. We solve partial differential equations for extrapolation using semi-Lagrangian approach with cubic Hermite interpolating polynomials. We use the time step restriction as was implemented in [F.Gibou et al., 2003].

Figure 2a shows two spheres of radius 0.2 whose centers offset by 0.05 units. 'T' inside the spheres is 0, where as outside it is -0.5. Diritchlet boundary conditions of $T = -0.5$ are considered at computational boundaries. PhysBAM's inbuilt fast marching method is used for reinitiation at every time step, and reinitialization is performed in a narrow band of $5\Delta x$. Grid considered for this test case is 50^3. Figure 2b shows the profile of zero level set at 180^{th} time step.

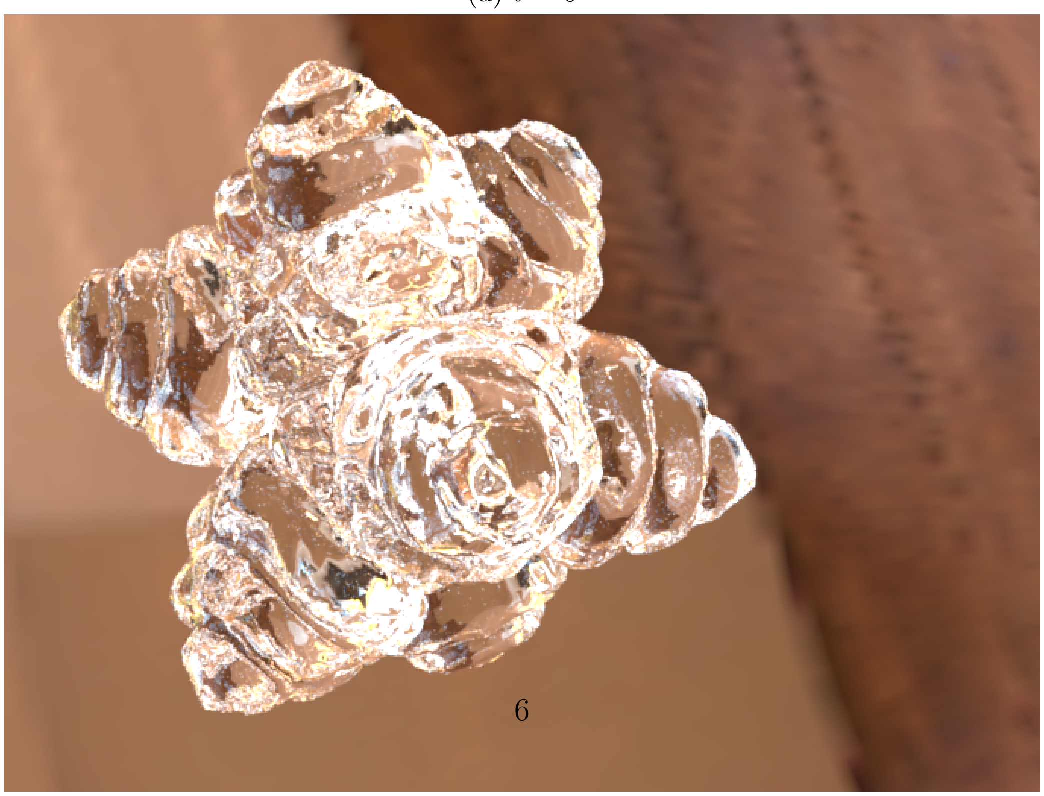
As a final test case, six spheres of radius 0.1 each are positioned whose centers are offset by 0.05 units on 100^3 grid is considered. Figures 3a and 3b show the initial and final profiles at $t = 180\Delta t$.

4 Conclusions and Future work

Gradient augmented level set approach is considered for interface advection. During the reinitialization step, we reported results by using fast marching method, where the gradient is computed numerically from the obtained signed distance function which is provided as input to gradient augmented approach, hence the name weak formulation of gradient augmented level set method is given to this work. The semi-Lagrangian approach followed for advection is also used for extrapolating temperature fields from either sides of the interface. Though not comparable to literature, our results show crystal like structures by using only constant extrapolation everywhere possible.

Executing test cases with linear extrapolations may lead to better results, i.e. comparable to literature [F.Gibou et al., 2003]. Scope to test our code with varying diffusion coefficients can also be considered.

(a) $t = 0$



(b) $t = 180\Delta t$

Figure 2: Application of Stephan problem to the interface initially defined by coalescence of two spheres.

(a) $t = 0$

(b) $t = 180\Delta t$

Figure 3: Application of Stephan problem to the interface initially defined by using six spheres whose centers are offset by 0.05 units.

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