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COMPARISON OF VARIOUS COUPLING METHODS FOR 1D DIFFUSION EQUATIONS WITH A ANALYTICAL SOLUTION OF TWO PHASE STEFAN PROBLEM

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Abstract. We implemented loose and tight coupling methods to understand thermal diffusion between ocean and ice by means of a simplified one-dimensional model set-up proposed by Stefan. A Stefan problem is a prototypical two-phase model that can used to model, for example, melting and freezing of water due to the transfer of heat fluxes between the two phases. We discretized heat fluxes using low order derivatives for loose coupling and higher order derivatives for tight coupling while fluxes are computed at the (moving) interface. Compared to a known reference solution the tight coupling method exhibits a lower error when compared to the loose coupling discretization. However, further numerical tests are required to analyze these coupling methods.

1 Introduction

The interaction of sea ice with ocean and atmosphere through the exchange of heat, moisture and momentum is one of the most important interactions in climate models. Especially, in the polar regions, sea ice forms an interface between ocean and atmosphere. Thermal process such as downward radiation, turbulent heat flux from the atmosphere, the oceanic heat flux and dynamical processes such as wind stress, ocean ice stress and internal ice stress influence the sea ice distribution. This study mainly focuses on the sea ice thermodynamics, namely growth and melt through ice-ocean interaction. The relationship between sea ice melt and the heat supplied to the upper ocean from the atmosphere is explained in [6]. This study also suggests that during the ice melt season, the upper ocean and sea ice are thermodynamically strongly coupled. The growth and decay of sea ice affects the global thermohaline circulation and the intensity of oceanic deep convection [2].

The implementation of the sea ice component is a major issue during the development of any earth system model (ESM). In some ESMs, the ocean is coupled directly to the atmosphere over the sea ice, in which the ice model sends a sea ice fraction to the ocean and, in turn, the ocean sends information about new ice growth to the ice model. It is also common for ESMs to incorporate a subset of the sea ice thermodynamics into the atmosphere component where it is computed on the atmosphere grid with the atmosphere's physics time step. The rest of the sea ice processes lies within the ocean component and are solved on the ocean grid with the ocean's time step [5]. While there have been some major advances in the most complex sea ice models during the past decade, the processes of atmosphere-ice-ocean interaction are still only crudely understood and it is therefore not clear if they are realistically represented in the models. It is also very challenging to assess the quality of sea ice simulations in coupled climate models against the observed sea ice evolution.

Some of the differences between observations and models could be due to limited observations and inaccurate coupling methods between the ocean and sea ice models. In ESMs the sub-components of a climate model are coupled with each other at their boundaries through couplers. The main function of a coupler is to interpolate the coupling fields and provide input to the sub-components. However, it is still unclear if this coupling strategy provides a consistent framework for coupling components of climate models. Hence there is a need to understand the various coupling methods. Therefore, the motivation of the present study is to understand what we call loose and tight coupling methods (see below). We do this for thermodynamics, namely on melting and freezing of ice by exchanging temperatures and heat fluxes at the interface and compare the results with an analytical solution of the two phase Stefan problem. The spirit of this work lies in taking a different point of view: instead of coupling various subsystems of a complex system we look at the system as a whole and rather consider decoupling strategies into less complex model parts whose dynamics consistently reflect the dynamics of the whole system.

The Stefan problem was among the first mathematical models to study heat distribution in a phase changing medium [8]. Examples of Stefan problems include the melting of ice, solidification, fluid flow in porous media, and shock waves in gas dynamics. In this study, we consider the example of diffusion of heat in the melting of ice where the melting rate is based on the temperature gradients at the interface. This ad-hoc procedure is very simple, yet energy conserving. The Neumann method [3] is used to obtain an analytical solution for the two phase Stefan problem and is used as a reference to our study. For simplicity, the phase change temperature (interface temperature) between the two phases in our Stefan problem is assumed to be constant. More realistic models for the temperature at the ice-ocean interface are surveyed in [4].

Loose coupling was implemented in [1] to couple separate computations of one-dimensional thermal diffusion in liquid (ocean) and solid (ice) domains. In loose coupling, low order derivatives are used to discretize heat fluxes at the interface. However, the accuracy of the solution is dependant on the width of the subdomain overlap of the models [7]. In order to increase the overlap at the interface, we implemented a tight coupling in addition to loose coupling where we use higher order derivatives to compute fluxes at the interface. Here we compare our solution of coupling methods to an analytical solution of two phase Stefan problem allowing for a rigorous comparison.

The organization of the paper is as follows. In Section 2, a two phase Stefan problem and its analytical solution are described. Section 3 describes the loose and tight coupling methods whereas Section 4 shows numerical tests. In Section 5 we discuss the results.

2 Model description of Two-phase Stefan Problem

A Stefan Problem is a specific type of a free boundary value problem for a partial differential equation for the distribution of heat in a phase changing medium. The Stefan problem is widely referenced in sciences where moving boundaries are considered. An example is the diffusion of heat in the melting of ice where melting causes the phase boundary of the ice to change position.

Consider a domain $\Omega = [0, X]$ in which the initial state of the material is assumed to be solid. We denote the temperature at the point x at time t by $u(x,t)$. A constant liquid temperature u_l which is less than melting temperature u_m is imposed at $x = 0$ resulting in an increase of temperature to reach the melting point causing liquid to appear in the domain. Let $s(t)$ be the point separating the two phases which determines the (initial) position of the interface. Movement of the interface is based on the temperature gradients of solid and liquid phase. The interface temperature is assumed to be constant, for simplicity. Two phase Stefan problem is mathematically expressed as heat conduction in liquid region

$$\frac{\partial u}{\partial t} = k_l \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < s(t), \quad t > 0 \tag{1}$$

and heat conduction in solid region

$$\frac{\partial u}{\partial t} = k_s \frac{\partial^2 u}{\partial x^2}, \quad x > s(t), \quad t > 0 \tag{2}$$

where $k_l > 0$ and $k_s > 0$ are constant but possibly different diffusion coefficients for each phase.

The temperature at the interface is given by

$$u(s(t), t) = u_m, \quad t > 0 \tag{3}$$

where u_m is the melting temperature which is assumed to be constant in time. The position of the interface $s(t)$ is determined by the jump condition also called Stefan condition which satisfies the principle of conservation of energy:

$$\rho L \frac{ds}{dt} = k_s \frac{\partial u}{\partial x} - k_l \frac{\partial u}{\partial x}, \quad x = s(t), \quad t > 0 \tag{4}$$

where L and ρ are latent heat and density respectively and are assumed to be constant. The initial condition is given by

$$u(x,0) = u_s < u_m, \quad x > 0, \quad s(0) = 0 \tag{5}$$

where u_s is the solid temperature which is also assumed to be constant. Boundary conditions are given by

$$\begin{aligned} u(0,t) &= u_l > u_m, \quad t > 0 \\ u(x,t) &= u_s \quad t > 0 \end{aligned} \tag{6}$$

where u_l is the liquid temperature which is also assumed to be constant.

2.1 An Analytical Solution

An analytical solution of the above two-phase Stefan problem was obtained by Neumann [3] in terms of a similarity variable ξ given by

$$\xi = \frac{x}{2\sqrt{k_l}}\,. \tag{7}$$

The solution for the interface position can be written as

$$s(t) = 2\lambda\sqrt{k_l t} \tag{8}$$

the temperature in the liquid phase reads

$$u(x,t) = u_l - (u_l - u_m)\frac{\operatorname{erf}(\frac{x}{2\sqrt{k_l t}})}{\operatorname{erf}(\lambda)} \tag{9}$$

and the temperature in the solid phase as

$$u(x,t) = u_s + (u_m - u_s)\frac{\operatorname{erfc}(\frac{x}{2\sqrt{k_s t}})}{\operatorname{erfc}(v\lambda)} \tag{10}$$

where $\operatorname{erf}(\xi)$ denotes the Gaussian error function and $\operatorname{erfc}(\xi)$ denotes the complementary error function

$$\begin{aligned} \operatorname{erf}(\xi) &= \frac{2}{\sqrt{\pi}}\int_0^{\xi} \exp(-\theta^2)d\theta \\ \operatorname{erfc}(\xi) = 1 - \operatorname{erf}(\xi) &= \frac{2}{\sqrt{\pi}}\int_x^{\xi} \exp(-\theta^2)d\theta \end{aligned} \tag{11}$$

The basic properties of these functions are

$$\begin{aligned} \operatorname{erf}(0) = 0\,, &\qquad \operatorname{erf}(\infty) = 1\,, \\ \frac{d\operatorname{erf}(\xi)}{d\xi} &= \frac{2}{\sqrt{\pi}}\exp(-\xi^2) > 0\,, \quad \text{and} \\ \frac{d^2\operatorname{erf}(\xi)}{d\xi^2} &= -2\xi\frac{d\operatorname{erf}(\xi)}{d\xi} = \frac{-4\xi}{\sqrt{\pi}}\exp(-\xi^2)\,. \end{aligned}$$

The parameter λ in equations (8)-(10) is the solution to the transcendental equation

$$\lambda\sqrt{\pi} = \frac{\mathrm{St}_l}{\exp(\lambda^2)\operatorname{erf}(\lambda)} - \frac{\mathrm{St}_s}{v\exp(v^2\lambda^2)\operatorname{erf}(v\lambda)} \tag{12}$$

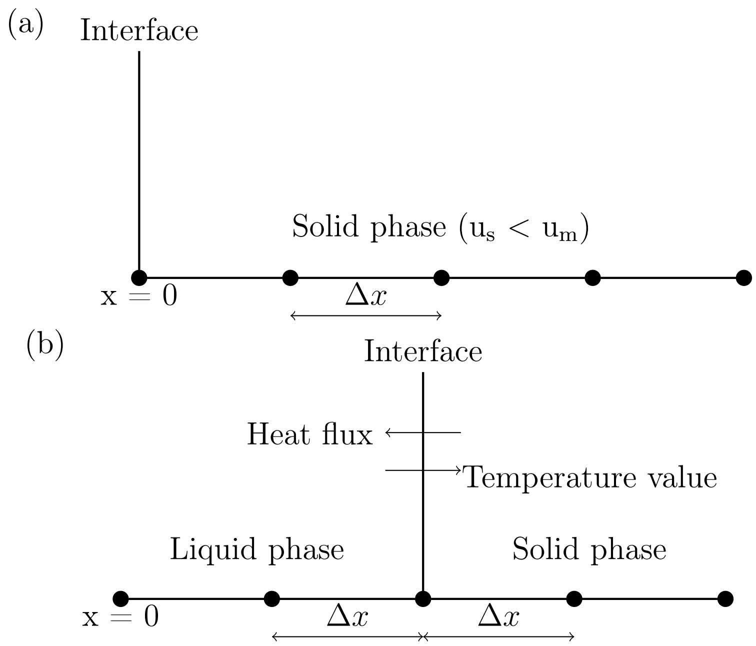


Figure 1: 1D Schematic representation of coupling methods at (a) t= 0 and (b) t> 0.

where $\text{St}_l = \frac{C_l(u_l - u_m)}{L}$ and $\text{St}_s = \frac{C_s(u_m - u_s)}{L}$ are the Stefan number for the liquid and the solid, respectively. The parameters $v = \sqrt{\frac{k_l}{k_s}}$, C_l and C_s are the heat capacities at constant pressure for liquid and solid, respectively, and are assumed to be constant.

3 Coupling methods

We consider the same heat equations as in (1) and (2), but the interface condition in these coupling methods are different from Stefan's condition (4). For simplicity, the interface temperature in a Stefan problem is assumed to be constant. We, on the other hand, implement loose and tight coupling methods in which we compute the temperature at the interface by exchanging temperature values from liquid domain and heat fluxes from solid domain [1]. The solutions to our different coupling methods are compared to the analytical solution of the Stefan problem.

Figure 1(a) shows the initial condition of the model, where the material is solid and the interface is $x = 0$. Figure 1(b) represents the movement of the interface based on new interface temperature. The interface temperature is computed by exchanging temperature values from the solid domain for the computation of liquid domain, and heat fluxes for the computation of the liquid domain from the solid domain. If this interface temperature exceeds the melting point of ice, the interface temperature is set to that value and the excess energy is considered to melt the ice.

The heat equation for liquid and solid domains is same as (1) and (2). The coupling equation at the interface is

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}(k_s \frac{\partial u}{\partial x} - k_l \frac{\partial u}{\partial x}) \,. \tag{13}$$

In the following subsections, we elaborate on the implementation of loose and tight coupling methods.

3.1 Loose Coupling

The numerical algorithm for determining u_i^{n+1} for the liquid is

$$\frac{(u_i^{n+1} - u_i^n)\Delta x}{\Delta t} = \frac{k_l}{\Delta x}(u_{i+1}^n - 2u_i^n + u_{i-1}^n), \quad (i \leq ib) \tag{14}$$

The corresponding numerical algorithm for determining u_i^{n+1} for the solid is

$$\frac{(u_i^{n+1} - u_i^n)\Delta x}{\Delta t} = \frac{k_s}{\Delta x}(u_{i+1}^n - 2u_i^n + u_{i-1}^n), \quad (i \geq ib) \tag{15}$$

while the numerical algorithm to determine interface temperature u_{ib}^{n+1} is

$$\frac{(u_{ib}^{n+1} - u_{ib}^n)\Delta x}{\Delta t} = -q_w - \frac{k_l}{\Delta x}(u_{ib}^n - u_{ib-1}^n), \quad (i = ib) \tag{16}$$

where q_w is the heat flux specified at the interface, is given by

$$q_w = -\frac{k_s}{\Delta x}(u_{ib+1}^n - u_{ib}^n)\ . \tag{17}$$

To summarize the communication between the two calculations for $i \leq ib$ and $i \geq ib$, at each time step there is an exchange of data, with the program performing the calculation for $i \leq ib$ supplying the temperature value of u_{ib}^n to the other program performing the calculation for $i \geq ib$, while the program performing the calculation for $i \geq ib$ supplies heat flux q_w to perform the calculation for $i \leq ib$.

If u_{ib}^{n+1} exceeds the melting temperature u_m, the interface moves to the right of domain representing melting of solid. If u_{ib}^{n+1} is less than the melting temperature, the interface moves to the left of domain, representing freezing of liquid.

3.2 Tight coupling

In order to achieve higher order accuracy, higher order approximations of the derivatives are used. We consider forward in time and centered difference in space for discretizing the heat equation. We use fourth order central difference approximations for first order derivatives to calculate the heat flux at the interface. These approximations use five point stencils in one dimension.

The numerical algorithm for determining u_i^{n+1} for the liquid is

$$\frac{\Delta x}{\Delta t}(u_i^{n+1} - u_i^n) = \frac{k_l}{\Delta x}(u_{i+1}^n - 2u_i^n + u_{i-1}^n)\ , \quad (i \leq ib) \tag{18}$$

while the corresponding numerical algorithm to determine u_i^{n+1} for the solid is

$$\frac{\Delta x}{\Delta t}(u_i^{n+1} - u_i^n) = \frac{k_s}{\Delta x}(u_{i+1}^n - 2u_i^n + u_{i-1}^n), \quad (i \geq ib)\ . \tag{19}$$

The numerical algorithm to determine interface temperature u_{ib}^{n+1} is

$$\frac{\Delta x}{\Delta t}(u_{ib}^{n+1} - u_{ib}^{n}) = -q_w - \frac{k_l}{\Delta x}(u_{ib-2}^{n}/12 - 2u_{ib-1}^{n}/3 - 2u_{ib+1}^{n}/3 + u_{ib+2}^{n}/12), \quad (i = ib) \tag{20}$$

where q_w denotes the heat flux specified at the interface given by

$$q_w = -\frac{k_s}{\Delta x}(u_{ib-2}^{n}/12 - 2u_{ib-1}^{n}/3 - 2u_{ib+1}^{n}/3 + u_{ib+2}^{n}/12)$$

If $u_{ib}^{n+1} \geq u_m$, the interface moves to the right of domain representing melting of solid. If $u_{ib}^{n+1} < u_m$, the interface moves to the left of domain, representing freezing of liquid. In the following section, we validate the results of loose and tight coupling methods to analytical solution of two phase Stefan problem.

4 Numerical tests

In order to investigate the relative error between the analytical solution and the coupling methods, we consider L^2-error norm, i.e., the root mean square error, for the temperature. Let $u_{\text{analytical}}$ be the analytical solution of the Stefan problem and u_{coupling} be the solution for loose and tight coupling methods. The relative L^2-error norm at time t^n for nx (number of grid points) is given by

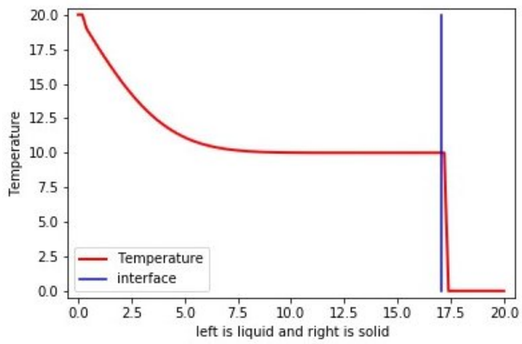
$$\text{Relative error} = \frac{\sum_{i=1}^{nx} |u_{i,\text{analytical}} - u_{i,\text{coupling}}|^2}{\sum_{i=1}^{nx} |u_{i,\text{analytical}}|^2} \tag{21}$$

Figure 3 shows the relative error for L^2 norm for temperature between the analytical solution of two phase Stefan problem and solution of loose and tight coupling methods.

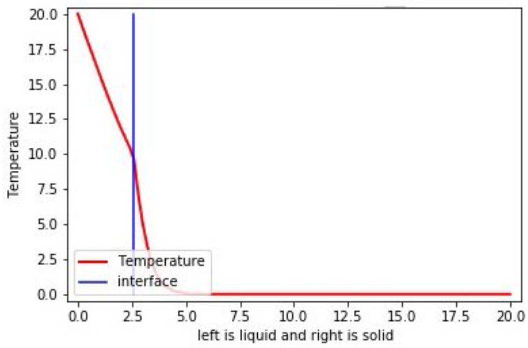
5 Results and Discussion

Figure 1 shows that the initial state of the material is solid. We impose a liquid temperature u_l which is greater than melting temperature u_m at $x = 0$. This results in an increase of temperature from the side $x = 0$, and when the temperature reaches the melting point, the material starts melting into liquid. The interface separates the two phases, where there is an exchange of temperature values from the liquid domain and heat fluxes from the solid domain. In Stefan problem and coupling methods, the heat equations for liquid and solid, initial and boundary conditions are the same. But the equation at the interface for Stefan problem (Stefan condition) is different from coupling methods. In the Stefan problem, the interface temperature is fixed for simplicity and Stefan's condition represents the movement of the interface based on the temperature gradients at the interface. However, assuming the fixed temperature at the interface is not realistic, and as a result, we compute the temperature at the interface in coupling methods.

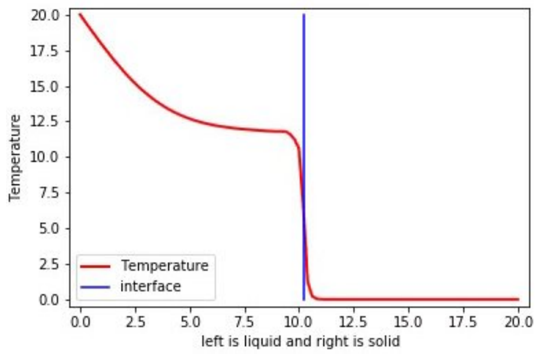
We implemented loose and tight coupling methods to couple thermal diffusion equation for liquid and solid domains. The two domains are coupled by exchanging temperature values (Dirichlet type) and heat fluxes (Neumann type) at the interface. The heat equations



(a)



(b)



(c)

Figure 2: (a) Analytical solution of two phase Stefan problem, (b) solution of loose coupling, (c) solution of tight coupling at $t \approx 1$. The red line represents temperature and the blue line represents the position of the interface.

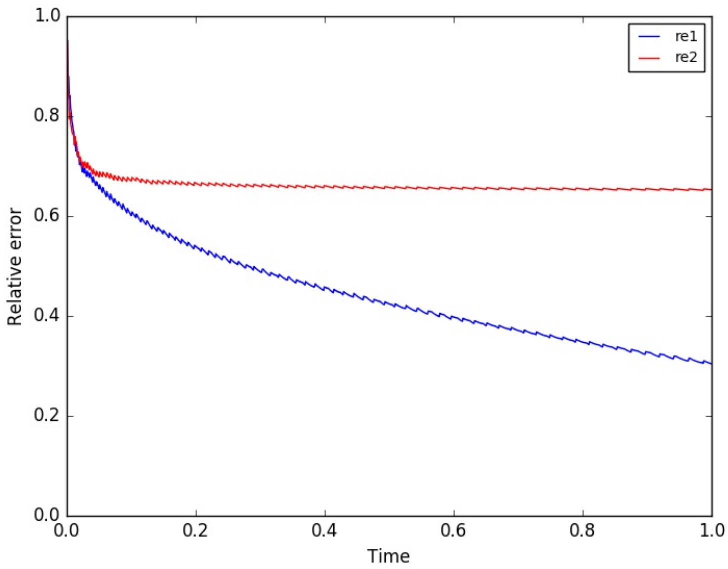


Figure 3: re1 represents the relative error in the L^2-norm between the analytical solution of two phase Stefan problem and the solution of tight coupling method. re2 represents the relative error in the L^2-norm between the analytical solution of two phase Stefan problem and solution of the loose coupling method.

for liquid and solid domains in loose and tight coupling methods are discretized by forward in time and centered difference in space. For the calculation of fluxes at the interface, we considered low order derivatives for loose coupling and higher order derivatives for tight coupling. These coupling methods compute temperature at the interface at each time step, but the interface position does not change. We consider the analytical solution of two phase Stefan problem for comparison since it yields energy conserving and consistent solution. In order to move the interface position in coupling solutions to compare to the analytical solution, we consider index ib to move to the right side of the domain by one grid point, representing melting if the interface temperature is greater than melting temperature. If the interface temperature is less than the melting temperature, we consider index ib to move to left side of the domain by one grid point, representing freezing of liquid.

Figure 2a represents the analytical solution of two phase Stefan problem. Red lines represent the diffusion of temperature and the blue line represent the position of the interface. We observe that the position of interface is $x = 17.5$. Figure 2b represents the solution of loose coupling, and the interface position is at $x = 2.5$, while Figure 2c represents the solution of tight coupling and the interface is at $x = 10$. From the results, we observe that the interface in loose and tight coupling solutions moves to the right side of the domain representing melting of solid. We also observe that the solution with tight coupling looks closest to the analytical solution when compared to the solution of loose coupling. Furthermore, Figure 3 shows that the relative error for L^2-norm between the analytical solution of two phase Stefan problem and solution for tight coupling method shows less error when compared to the solution with loose coupling method. This may be due to the large overlap in tight coupling. However, this study requires further analysis for loose and tight coupling methods and also needs realistic representation to move the interface in coupling methods.

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REFERENCES

[1] Giles, M.B. *Stability analysis of numerical interface conditions in fluid structure thermal analysis*, Int. J. Num. Meth. Fluids, **25**: 421–436 (1997)

[2] Komuro, Y. and Hasumi, H., *Effects of surface freshwater flux induced by sea ice transport on the global thermohaline circulation*, J. Geophys. Res., **108**: 3047 (2003)

[3] Neumannn, F., *Die Partiellen Differentialgleichungen der Mathematischen Physik*, Reimann–Weber, Vol. II. (1912)

[4] Notz, D., *Challenges in Simulating Sea Ice in Earth System Models*, WIREs. Clim. Change, **3**: 509–526 (2012)

[5] Notz, D. and Bitz, C.M., *Sea ice in Earth system models*, Sea Ice. 3rd. ed. pp. 304-329 (2016)

[6] Ohshima, K.I., Yoshida, K., Shimoda, H., Wakatsuchi, M., Endoh, T. and Fukuchi, M., *Relationship between the upper ocean and sea ice during the Antarctic melting season*, J. Geophys. Res., **103**: 7601–7615 (1998)

[7] Samarskii, A. and Vabishchevich, P., *Domain decomposition methods for parabolic problems*, Eleventh International Conference on Domain Decomposition Methods, pp. 341–347 (1999)

[8] Stefan, J., *Über die Theorie der Eisbildung, inbesondere über die Eisbildung im Polarmeer*, Ann. Chem. Phys., **42**: 269–286 (1891)