Finite Element Implementation of Nonlinear Heat Equation in Enthalpy Formulation using ALBERT(A).

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-

abstract

In this paper we describe an implementation of approximate solution to the enthalpy formulation of the Stefan problem.

We allow the thermal properties to have a space and temperature dependence. The algorithm is not explicit in the time variable and hence the stability condition on the time steps is not too severe.

The main aim of this note is program documentation of solving nonlinear heat equation implemented in ALBERT(A) an adaptive finite element method package.

Keywords: Nonlinear Heat Problem, Stefan Problem, Enthalpy Formulation, Kirchoff Transformation, ALBERT(A)

MSC : Primary 65H10, 65M05;Secondary 35K55, 76S05

Nomenclature :

Θ	Temperature
$H = H(\Theta)$	Enthalpy
$\beta(\Theta) = u$	'Generalized' Temperature
Θ_r	Reference Temperature
$c(\Theta)$	heat capacity (Temperature dependent)
$\rho(\Theta)$	density (Temperature dependent)
$k(\Theta)$	heat conductivity (Temperature dependent)
ν	Normal Vector
Θ_m	melting temperature, exactly dependent on Phase diagram which dependent on Temperature

1 Introduction

Many industrial (thermal) process involving change of phases. This problem is well known as Stefan's problem, for example :[2]

1. Crystal Growth
2. Freeze Drying
3. Moisture diffusion
4. Laser Ablation

This report documenting an implementation of Finite Element solver for Stefan's problem in ALBERT, later released as ALBERTA [10], a Finite Element toolbox with hierarchical spatial adaptivity. However, we pose the problem in a general setting for a class of nonlinear heat equation which subsumed Stefan's problem instead. Hence we started with a model posed as a fully non-linear heat equation.

2 Governing Equations

Let $\Omega \in \mathbb{R}^2, T > 0, Q := \Omega \times (0, T)$

We concerned with non-linear heat equation of the following in Ω :

$$c(\Theta)\rho(\Theta)\frac{\partial\Theta}{\partial t} = \nabla \bullet (k(\Theta)\nabla\Theta) + f(x, t) \quad (1)$$

On the boundary $\partial\Omega = \Gamma_D \cup \Gamma_N, \Gamma_D \cap \Gamma_N = \emptyset$, we set the following condition on Temperature :

$$\begin{aligned} \Theta(x, t) &= \Theta_D(x), \text{ for } x \in \Gamma_D \subset \partial\Omega, & (\text{Dirichlet condition}) \\ -k(\Theta)\nabla\Theta(x, t) \bullet \nu &= \Theta_N(x), \text{ for } x \in \Gamma_N \subset \partial\Omega, & (\text{Neumann condition}) \end{aligned}$$

Initially, over Ω , we set for Temperature an initial condition :

$$\Theta(x, 0) = \Theta_0(x), \text{ for } x \in \Omega$$

We introduce two transformation of variable to remove temperature dependency in the coefficients as follows :

$$\begin{aligned}
H(\Theta) &= \int_0^\Theta c(\zeta)\rho(\zeta)d\zeta, & (\text{Enthalpy}) \\
u = \beta(\Theta) &= \int_0^\Theta k(\xi)d\xi, & (\text{Kirchoff Transformation})
\end{aligned}$$

See [12], also[8], for the arguments behind this transformation and some physical interpretation.

Assuming that β invertible, then we have the following relation :

$$\Theta = \Theta(u) = \beta^{-1}(u)$$

Note this is true for the case of most physical problem, since $k(\zeta)$ is non-negative real-valued, hence β is a monotonic function.

The non-linear heat equation (1) after Kirchoff's transformation in Enthalpy formulation:

$$\frac{\partial H}{\partial t} = \Delta u + f(x, t) \quad (2)$$

with corresponding boundary conditions ;

$$\begin{aligned}
u(x, t) &= \int_0^{\Theta_D(x, t)} k(\xi)d\xi, \text{ for } x \in \Gamma_D \\
&= u_D \\
\frac{\partial}{\partial \nu} u(x, t) &= \int_0^{\frac{\partial}{\partial \nu} \Theta(x, t)} k(\xi)d\xi, \text{ for } x \in \Gamma_N \\
&= u_N
\end{aligned}$$

and initial conditions :

$$\begin{aligned}
H(x, 0) &= \int_0^{\Theta(x, 0)} c(\zeta)\rho(\zeta)d\zeta, \text{ for } x \in \Omega \\
&= H_0
\end{aligned}$$

2.1 Stefan Problem

Here, we are more interested in the case where a substance undergoes a change of phases at the temperature $\Theta = \Theta_m$, with temperature dependent specific heat on each respective phases :

$$c(\Theta) = \begin{cases} c_s(\Theta), & \Theta < \Theta_m \\ c_l(\Theta), & \Theta_m \leq \Theta \end{cases} ,$$

then the enthalpy may be written as:

$$H(\Theta) = \begin{cases} \int_0^\Theta c_s(\zeta) \rho_s(\zeta) d\zeta, & \Theta < \Theta_m \\ H(\Theta_m^-) + \lambda + \int_{\Theta_m}^\Theta c_l(\zeta) \rho_l(\zeta) d\zeta, & \Theta_m \leq \Theta \end{cases},$$

where: $H(\Theta_m^-) = \lim_{\delta \rightarrow 0^-} H(\Theta_m + \delta)$

Due to presence of latent heat, observe that there exist a jump discontinuity in Enthalpy function. In practice, we need to regularize the singularity. A regularization trick was suggested by [6] which adopted by [4] to solve Stefan problem using moving finite element.

The regularized enthalpy is of the form :[4]

$$H(\Theta) = \begin{cases} \int_0^\Theta c_s(\zeta) \rho_s(\zeta) d\zeta + \frac{\lambda}{2} \exp\left(-\frac{|\Theta - \Theta_m|}{\epsilon^-}\right) & \Theta < \Theta_m \\ H(\Theta_m^-) + \frac{\lambda}{2} + \int_{\Theta_m}^\Theta c_l(\zeta) \rho_l(\zeta) d\zeta - \frac{\lambda}{2} \exp\left(-\frac{|\Theta - \Theta_m|}{\epsilon^+}\right), & \Theta_m \leq \Theta \end{cases}$$

To ensure continuous differentiability of $H(\Theta)$ at Θ_m , we requires:

$$c_s(\Theta_m^-) - c_l(\Theta_m^+) = \frac{\lambda}{2} \left(\frac{1}{\epsilon^+} - \frac{1}{\epsilon^-} \right)$$

In [7], a much more simpler regularization were proposed, the proposed regularization is of the following form:

$$H(\Theta) = (\Theta - \Theta_m) + \frac{\lambda}{2} \left(1 + \frac{(\Theta - \Theta_m)}{\sqrt{(\Theta - \Theta_m)^2 + \epsilon}} \right)$$

Another regularization is via Apparent Heat Capacity (AHC) which used in [3], where the regularization is using linear approximation to smooth the jump. We observe that the earlier two regularization type are more favorable during our computation runs compared to the AHC, since we able to use smaller regularization gap : $\epsilon = (\epsilon^+ + \epsilon^-)$, which means resolving the interval of discontinuity more accurately at the jump. Hence from now on we might use one of the two earlier type of enthalpy regularization.

3 Finite Element Discretization

Let : $[0, T] := [0 < t_1 < t_2 < \dots < t_N = T]$

$$\tau_n = t_n - t_{n-1} \quad k = 1, \dots, N$$

Let $H_D^1(\Omega) = \{u; u, \frac{\partial u}{\partial x_i} \in L^2(\Omega), u|_{\Gamma_D} = 0\}$

Using implicit Euler scheme in time, the time discrete problem :

$$\frac{1}{\tau_n} (H^n - H^{n-1}) - \Delta \tilde{u}^n = f^{n-1}$$

Write :

$$u^n = (\tilde{u}^n - \tilde{u}_D) \in H_D^1(\Omega)$$

The weak problem :

$$\begin{aligned} F(u^n; v) &= \frac{1}{\tau_n} \int_{\Omega} H^n v \\ &+ \int_{\Omega} \nabla u^n \nabla v \\ - \{ \frac{1}{\tau_n} \int_{\Omega} H^{n-1} v - \int_{\Omega} \nabla \tilde{u}_D \nabla v \}, \forall v \in H_D^1(\Omega) \\ F(u^n; v) &= \int_{\Omega} f^{n-1} v, \forall v \in H_D^1(\Omega) \end{aligned}$$

3.1 Finite Element Implementation in ALBERT

The implementation of heat equation case that accompanied ALBERT source codes (see section **3.3.** in [9]) were modified to solve the Stefan problem. Please consult the corresponding section, with a word of warning that the provided case accompanied the software is slightly different in words with the case described in the Manual [9]. However, logically the description in [9] is still valid.

Here, description of main modification are made. Details on the `main()` program concerning time/space adaptation is not discussed, please refer to the corresponding section on heat equation case in [9].

3.1.1 Global Variables

fe_space: a pointer to the finite element space chosen, it is initialized on the first call of `main()`

u.h: a pointer to a DOF vector storing the coefficients of the discrete solution for (dependent) variable u ('Generalized' Heat), it is initialized on the first call of `main()`

u.old: a pointer to a DOF vector storing the coefficients of the discrete solution for previous step $U^{(n)}$, it is initialized on the first call of `main()`

T.h: a pointer to a DOF vector storing the coefficients of the discrete solution for (dependent) variable Θ (Temperature), it is initialized on the first call of `main()`

T.old: a pointer to a DOF vector storing the coefficients of the discrete solution for previous step $\Theta^{(n)}$, it is initialized on the first call of `main()`

H.h: a pointer to a DOF vector storing the coefficients of the discrete solution for (dependent) variable H (Enthalpy), it is initialized on the first call of `main()`

H.old: a pointer to a DOF vector storing the coefficients of the discrete solution for previous step $H^{(n)}$, it is initialized on the first call of `main()`

f.h: a pointer to a DOF vector storing the load vector; it is initialized on the first call of `main()`

A.matrix: a pointer to DOF matrix storing the stiffness matrix; it is initialized on the first call of `main()`

MassD: a pointer to DOF vector storing the diagonal mass matrix; it is initialized on the first call of `main()`

A global pointer to the `ADAPT_INSTAT` structure is used for access in the `build()` and `estimate()` routines.

3.1.2 Functions for leaf data

See section 3.3.2 in [9]

3.1.3 Data of the differential equation

Data for the Stefan problem are the initial values of the Enthalpy H_0 , right hand side f , and boundary values u_D . Note that, all of these values are dependent on temperature variable, $\Theta(x, y, t)$. When the true solution for the temperature is known, $\Theta(x, y, t)$, hence we will now the exact solutions of Enthalpy H and the Kirchoff-transformed of temperature variable, u .

3.1.4 Time discretization

The model implementation uses Euler implicit time scheme. Initial data is interpolated on the initial mesh,

$$\Theta_0 = I_0 \theta_0; \quad H_0 = I_0 H_0$$

The solution $U^{n+1} \approx u(., t_{n+1})$ and $H^{n+1} \approx H(., t_{n+1})$ is given by $U^{n+1} \in I_{n+1}g(., t_{n+1}) + X_{n+1}^o$ and $H^{n+1} \in X_{n+1}^o$ such that :

$$\frac{1}{\tau_{n+1}}(H^{n+1}, \Phi) + (\nabla U^{n+1}, \nabla \Phi) = \frac{1}{\tau_{n+1}}(H^n, \Phi) + (f(., t_{n+1}), \Phi), \quad \forall \Phi \in X_{n+1}^o$$

Note that, we don't deal with temperature variable directly during computations. We recover the temperature from Enthalpy or it's Kirchoff transformed variables.

3.1.5 Initial data interpolation

In our problems, the initial data required is Enthalpy, H_0 , rather than initial Temperature, hence it requires transformation from T_0 to H_0 . Initial data T_0 is just interpolated on the initial mesh, and H_0 obtained through function evaluation, thus the `solve()` entry in `adapt_instat->adapt_initial` will point to a routine `interpol_Data0()` and which implements this by the library interpolation routine. No `build()` routine is needed by the initial mesh adaptation procedure.

3.1.6 Assembly of the discrete system

Using matrix notation, the non-linear discrete problem can be written as :

$$\frac{1}{\tau_{n+1}}M(\Phi^{n+1}) + A\Phi^{n+1} = \frac{1}{\tau_{n+1}}M(\Phi^n) + F^{n+1}$$

Here, $M = (\Phi_i, \Phi_j)$ (up to Dirichlet boundary nodes) denotes the mass matrix and $A = (\nabla \Phi_i, \nabla \Phi_j)$ the stiffness matrix. Following the argument as given in the section **(3.3.6)** in [9], matrix-vector multiplication on the right hand side is realized through local contributions of each single element during assembly.

Most arguments in the section **3.3.6.** of [9] is still valid, with an exception that the global mass matrix is stored as a DOF vector, and the local mass operator is lumped before added to the global mass matrix.

```
static void assembly(DOF_REAL_VEC *u_h, DOF_REAL_VEC *H_h,
                    DOF_MATRIX *A_matrix, DOF_REAL_VEC *MassD,
```



```

        DOF_REAL_VEC *fh,
        REAL theta_step, REAL tau, REAL (*f)(const REAL_D),
        REAL (*u_D)(const REAL_D))
{
    FUNCNAME("assembly");
    static struct op_info *op_info = nil;
    static const REAL      **(*fill_a)(const EL_INFO *, void *) = nil;
    static void            *a_info = nil;
    static const REAL      **(*fill_c)(const EL_INFO *, void *) = nil;
    static void            *c_info = nil;

    static const DOF_ADMIN *admin = nil;
    static int             n;
    static const REAL      *(*get_H_loc)(const EL *, const DOF_REAL_VEC *, REAL *);
    static const DOF      *(*get_dof)(const EL *, const DOF_ADMIN *, DOF *);
    static const S_CHAR   *(*get_bound)(const EL_INFO *, S_CHAR *);

    TRAVERSE_STACK *stack = get_traverse_stack();
    EL_INFO         *el_info;
    FLAGS           fill_flag;
    const REAL      **a_mat, **c_mat;
    REAL            *f_vec, *m_vec;
    const QUAD      *quad ;
    int              i, j;

    quad = get_quadrature(DIM, 2*H_h->fe_space->bas_fcts->degree);

    /*****
    /*  init functions for matrix assembling
    /*****

    if (admin != H_h->fe_space->admin)
    {
        OPERATOR_INFO      o_info2 = {nil}, o_info0 = {nil};
        const EL_MATRIX_INFO *matrix_info;
        const BAS_FCTS      *bas_fcts = H_h->fe_space->bas_fcts;

```

```

admin          = H_h->fe_space->admin;

n = bas_fcts->n_bas_fcts;
get_dof        = bas_fcts->get_dof_indices;
get_bound      = bas_fcts->get_bound;
get_H_loc      = bas_fcts->get_real_vec;

if (!op_info)
    op_info = MEM_ALLOC(1, struct op_info);

o_info2.row_fe_space = o_info2.col_fe_space = H_h->fe_space;

o_info2.quad[2]      = quad ;
o_info2.LALt         = LALt;
o_info2.LALt_pw_const = true;
o_info2.LALt_symmetric = true;
o_info2.user_data    = op_info;

matrix_info = fill_matrix_info(&o_info2, nil);
fill_a = matrix_info->el_matrix_fct;
a_info = matrix_info->fill_info;

o_info0.row_fe_space = o_info0.col_fe_space = H_h->fe_space;

o_info0.quad[0]      = quad ;
o_info0.c            = c;
o_info0.c_pw_const   = true;
o_info0.user_data    = op_info;

matrix_info = fill_matrix_info(&o_info0, nil);
fill_c = matrix_info->el_matrix_fct;
c_info = matrix_info->fill_info;
}

op_info->tau_1 = 1.0/tau;

```

/*****

```

/* and now assemble the matrix and right hand side */
/*****

clear_dof_matrix(A_matrix);
dof_set(0.0,MassD) ;
m_vec = MassD->vec;
dof_set(0.0, fh);
f_vec = fh->vec;

fill_flag = CALL_LEAF_EL\vert FILL_COORDS\vert FILL_BOUND;
el_info = traverse_first(stack, H_h->fe_space->mesh, -1, fill_flag);
while (el_info)
{
    const REAL    *H_loc = (*get_H_loc)(el_info->el, H_h, nil);
    const DOF      *dof    = (*get_dof)(el_info->el, admin, nil);
    const S_CHAR   *bound  = (*get_bound)(el_info, nil);

/*****
/* initialization of values used by LALt and c */
/*****

    op_info->det    = el_grd_lambda(el_info, op_info->Lambda);

    a_mat = fill_a(el_info, a_info);
    c_mat = fill_c(el_info, c_info);

/*****
/* add_to A_matrix += a(psi_i,psi_j) */
/*****

    add_element_matrix(A_matrix, 1.0, n, n, dof, dof, a_mat, bound);

/*****
/* f += 1/tau*m(T_old,psi_i) */
/* add_to MassD += 1/tau*m(psi_i,psi_j) */
/*****

```

```

/*  theta_step = 1, i.e Backward Euler Step                                     */

    for (i = 0; i < n; i++)
    {
if (bound[i] < DIRICHLET)
{
    REAL val = 0.0;
    for (j = 0; j < n; j++)
    {
        m_vec[dof[i]] += c_mat[i][j] ; /* MassD += 1/tau*m(psi_i,psi_j) */
        val += c_mat[i][j]*H_loc[j];    /* Mass matrix multiplied to
                                           * T_old(local)                                */
    }
    f_vec[dof[i]] += val;
}
    }

    el_info = traverse_next(stack, el_info);
}

free_traverse_stack(stack);

L2scp_fct_bas(f, quad, fh); /* External forcing                               */

dirichlet_bound(u_D, fh, u_h, nil);/* apply boundary conditions for u */

return;
}

```

For each time step, the `build()` just calls `assembly()` routine described above, with evaluation times for right hand sides and boundary values adjusted to the next step.

```

static void build(MESH *mesh, U_CHAR flag)
{

```

```

FUNCNAME("build");

dof_compress(mesh);
MSG("%d DOFs for %s\n", fe_space->admin->size_used, fe_space->name);

eval_time_f = tm1 ;
eval_time_u_D = tm1;

assembly(u_h, H_h, A_matrix, MassD, f_h, theta_step, tau, f, u_D);

return;
}

```

The resulting non-linear systems solved using `nlsor()` routine. This is done via the `solve()` routine described in the section **3.1.7.** in [9].

```

/*****
/* solve(): solve the linear system, called by adapt_method_stat() */
*****/

static void solve(MESH *mesh)
{
    FUNCNAME("solve");
    static REAL      tol = 2.e-4 ;
    static int       max_iter = 100000, info = 2 ;
    static int       iter ;
    static REAL      omega = SORpar ;

    /* Solved using Non-Linear SOR for u_h ! */
    /*
    */

    iter = nlsor_s(A_matrix, MassD, f_h, nil, UtoH_Val,
                  u_h, omega, tol, max_iter, info);

    /* updates Temperature and Enthalpy at tm1 */
}

```

```

    UtoH_Vec(u_h,H_h) ;                               /* map u_h to H_h */
    InverseKirchoffTransformVec(u_h,T_h) ;             /* map u_h to T_h */

    return;
}

```

4 Nonlinear SOR

To solve the resulting non-linear discrete systems, we take resort using non-linear SOR[12]. Under several assumptions on H and u as functions of temperature, T , we express the discrete non-linear problem into the following form :

$$MH(U) + AU = b$$

with requirement : $a_{ii} > 0$, $m_{ii} > 0$, and let $\boxed{r_i(\zeta) = m_{ii}h(\zeta) + a_{ii}\zeta}$, under an assumption that it is invertible, with inverse function denoted by r_i^{-1} . Rewriting $MH(U) + AU = b$ into the form :

$$\begin{aligned}
 r_i(U_i) = b_i & - \sum_{i>j} \{a_{ij}U_j + m_{ij}H_j(U_j)\} \\
 & - \sum_{i<j} \{a_{ij}U_j + m_{ij}H_j(U_j)\}
 \end{aligned}$$

Due to diagonal format of the mass matrix, the nonlinear SOR algorithms proceed as follows[12]. Let $\omega \in [1, 2)$ be a provided relaxation parameter.

Iterates on $k = 1, \dots,$

$$\begin{aligned}
 U_i^{k+\frac{1}{2}} &= r_i^{-1} \left(b_i - \{ \sum_{i<j} a_{ij}U_j^{k+1} + \sum_{i>j} a_{ij}U_j^k \} \right) \\
 U_i^{k+1} &= (1 - \omega)U_i^k + \omega U_i^{k+\frac{1}{2}}
 \end{aligned}$$

until convergence reached.

Clearly, we need a root solver for scalar function $r(\zeta)$ for each iteration. We resolve this via Newton method.[12] The source code can be consulted in the appendix.

Note

As mentioned before, at a single iteration sweep, we have to find a root from $r(\zeta)$ for each degree of freedom. In the case the derivative of $r(\zeta)$ is not available, then during root finding iteration in the (scalar)-Newton iteration, finite-difference approximation of $r'(\zeta)$ are utilized. In our experience, this situation create a hindrance in some way to arrive to the root for a given tolerance, penalized computational time at each sweep. Hence, availability of analytical derivative of $r(\zeta)$ is quite desirable.

5 Numerical Test

Let $\Omega = (0, 1)^2$, $\Gamma_L = \{0\} \times [0, 1]$, $\Gamma_R = \{1\} \times [0, 1]$, $\Gamma_B = [0, 1] \times \{0\}$, $\Gamma_T = [0, 1] \times \{1\}$.

We set parameters for nlsor solver be : $\omega = 1.1$, tolerance = $2.0e - 4$, and the sor iteration will be bailed out after 10^5 iterations.

We consider three cases involving phase-change process in Ω for a material with $\rho_i = c_i = k_i = 1.0$. The material possessed a latent heat of value 1, i.e. $L = 1$, with solidification/melting temperature at zero. We apply zero Neumann boundary condition on $\Gamma_B \cup \Gamma_T$, i.e. insulation at top and bottom boundaries. While at the left boundary, Γ_L , we prescribed a constant temperature at $T|_{\Gamma_L} = -0.9$, while on the right boundary, Γ_R , we set a fix boundary temperature at $T|_{\Gamma_R} = 0.5$.

The domain Ω is triangulated using a fixed uniform grid consists of 16,389 triangles and 8,319 nodes. A constant time step $\Delta t = 0.0012$ are taken during the test. And the regularization parameter set at $\epsilon = 1.0e - 5$, for regularized enthalpy as suggested by Grosmann and Noack[7].

We consider three prescribed initial values for the problem, where for each initial values, the evolving process shows solidification process, melting, and both process occurs. In the first case, initially the material is in liquid phase at uniform temperature $T_0 = 0.5$, this case shows solidification process towards steady-state solution. In the second case, we set initially at solidification temperature $T_0 = 0$, which the process undergoes solidification and melting at the same time before reaching steady-state temperature. While the third case, we set initially the material is in solid phase at uniform temperature $T_0 = -0.5$, this case shows melting process towards steady-state

solution.

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APPENDIX A.

User supplied function.

To use the main driver, the user should provides geometrical data through Macro file, adaptivity infos through INIT file, and a file contains initial data, boundary conditions, and material parameter as user supplied function. One important function needed by the driver is a scalar-valued functions, taking a value in u , and map it to H , i.e. the following map :

$$H(u) = \int_0^{\beta^{-1}(u)} \rho(\zeta)c(\zeta)d\zeta$$

Essentially it is this map that holds material parameter function at once, to be passed to the main driver. In the case analytical expression of $H(u)$ is available, it is recommended to use non-linear solver which accepts function call for $\frac{d}{du}H(u)$. See commentary about this in the other appendix on non-linear SOR later.

The following code write up shows an example of implementation for the case of Silicon. In this write-up, we use the regularization given in [4], the user may found it is not difficult to replace the regularization expression for other expression, such as regularization given in [7]. Below, we utilize non-linear solver without calls to $\frac{d}{du}H(u)$:

```

/*****
/* ALBERT:    an Adaptive multi Level finite element toolbox using          */
/*            Bisectioning refinement and Error control by Residual          */
/*            Techniques                                                       */
/*****
/*
/*          authors: Alfred Schmidt and Kunibert G. Siebert                 */
/*                  Institut f"ur Angewandte Mathematik                     */
/*                  Albert-Ludwigs-Universit"at Freiburg                   */
/*                  Hermann-Herder-Str. 10                                  */
/*                  79104 Freiburg                                           */
/*                  Germany                                                  */
/*
/*          email:   alfred,kunibert@mathematik.uni-freiburg.de             */
*****/
```

```

/*      (c) by A. Schmidt and K.G. Siebert (1996-99)                                */
/*                                                                                      */
/*      modified by: A. D. Garnadi                                                    */
/*      Stiftung CAESAR                                                                */
/*      Crystal Growth Group                                                            */
/*      Friedensplatz 16                                                                */
/*      53111 Bonn                                                                    */
/*      (c) by A. D. Garnadi (2001)                                                    */
/*                                                                                      */
/*      Last updated: 30 August 2001                                                  */
/*****
/*****
/* solver for NonLinear Stefan problem~:                                           */
/*      \rho c_i T,t - div(k_i grad T) = 0, i=1,s */
/* using Implicit Euler Scheme                                                    */
/* The methods used are via Kirchoff Transformation :                             */
/*      u(T) = \int_0^T k(\xi) d\xi                                                 */
/* And Enthalpy functions:                                                         */
/*      H(T) = \int_0^T \rho(\xi) c(\xi) d\xi                                       */
/* such that the original problem turned into:                                     */
/*      H,t - delta u = 0                                                           */
/*****

#include <albert.h>

/*
#define AmplitudoL 20.0
#define AmplitudoR 10.0
*/
#define AmplitudoL 1000.0
#define AmplitudoR 2000.0
#define T_shift 0.0
#define T_melting 1685.0
#define phi_root 0.05254380387956843
#define epsReg 0.125
#define Latent 1800000.0

```

```

/*****
/* Silicon data */
*****/

REAL c_s= 900.0, c_l = 1000.0;
REAL rho_s = 2490.0 , rho_l = 2490.0 ;
REAL k_s = 22.0, k_l = 64.0 ;

/*****
/*          Enthalpy_Transformation, Inverse_Enthalpy_Transformation  */
*****/

/*****
/*          Inverse_Enthalpy_Transformation,                               */
/* Enthalpy_Transformation(Vector),Inverse_Enthalpy_Transformation(Vector) */
*****/

REAL EnthalpyTransformVal(const REAL T_val)
{
    FUNCNAME("EnthalpyTransformVal");

    REAL H_val ;
    REAL TL, TR ;
    REAL c_reg ;

    TL = T_melting - epsReg ; TR = T_melting + epsReg ;
    c_reg = 0.5*((c_s*rho_s + c_l*rho_l) + rho_s*Latent/epsReg);

    if(T_val<=T_melting)
        H_val = rho_s*c_s*T_val +
                rho_s*0.5*Latent*exp(-fabs(T_val - T_melting)/epsReg);
    else
        H_val = rho_s*c_s*T_melting + rho_l*c_l*(T_val - T_melting) +
                rho_s*0.5*Latent*( 1.0 - exp(-fabs(T_val - T_melting)/epsReg));

    return(H_val) ;
}

```

```

REAL InverseEnthalpyTransformVal(const REAL H_val)
{
    FUNCNAME("InverseEnthalpyTransformVal");

    REAL T_val;
    REAL rhoCeS, rhoCeL ;
    REAL TL, TR, HL, HR ;    REAL c_reg ;

    rhoCeS = rho_s*c_s ;    rhoCeL = rho_l*c_l ;

    TL = T_melting - epsReg ; TR = T_melting + epsReg ;
    c_reg = 0.5*((c_s*rho_s + c_l*rho_l) + rho_s*Latent/epsReg);

    HL = rhoCeS*TL ;    HR = rhoCeS*TL + c_reg*(TR-TL);

    if(H_val<HL)
        T_val = H_val/rhoCeS ;/* value of IET                                */
    else
    {
        if(HL<H_val<HR)
            T_val = (H_val - rho_s*c_s*TL)/c_reg + TL ;
        else
            T_val = (H_val - rho_s*c_s*TL - c_reg*(TR - TL))/rhoCeL ;
    }

    return(T_val) ;
}

/*****
/*          Kirchoff_Transformation, Inverse_Kirchoff_Transformation      */
*****/

REAL Heat_conductivity(const REAL T)
{
    FUNCNAME("Heat_conductivity");
    REAL k_val ;

```

```

    if(T<T_melting)
        k_val = k_s ;
    else
        k_val = k_l ;

    return(k_val) ;
}

REAL KirchhoffTransformVal(const REAL T_val)
{
    FUNCNAME("KirchhoffTransformVal");
    REAL x_val ;

    /* x_val = T_val ; */

    if(T_val<T_melting)
        x_val = k_s*T_val ;
    else
        x_val = k_l*(T_val - T_melting) + k_s*T_melting;

    return(x_val) ;
}

REAL InverseKirchhoffTransformVal(const REAL u_val)
{
    FUNCNAME("InverseKirchhoffTransformVal");
    REAL T_val ;

    /* value of IKT */
    REAL ksTm = k_s*T_melting;

    if(u_val<ksTm)
        T_val = u_val/k_s ;
    else
        T_val = (u_val - k_s*T_melting)/k_l + T_melting ;
}

```

```

    return(T_val) ;
}

/*****
/* problem data: right hand side, boundary values */
*****/

REAL eval_time_T ;
REAL eval_time_T_D ;

/* NEEDED: for T boundary values, not optional */
REAL T_D(const REAL_D x)/* boundary values for T, not optional*/
{
    FUNCNAME("T_D");

    REAL T_val, phase_pos ;
    REAL Kappa_s = k_s/c_s, Kappa_l = k_l/c_l, ratioK ;
    REAL erfPhi = erf(phi_root), erfcPhi;
    REAL sqrt_1S, sqrt_1L ;
    sqrt_1S = 0.5/sqrt(Kappa_s*eval_time_T_D) ;
    sqrt_1L = 0.5/sqrt(Kappa_l*eval_time_T_D) ;
    ratioK = sqrt(Kappa_s/Kappa_l) ;

    erfcPhi = erfc(ratioK*phi_root) ;

    phase_pos = 2.0*phi_root*sqrt(Kappa_s*eval_time_T_D);

    {
        if(x[0]>= 0.5)
            T_val = AmplitudoR + T_shift ;
        else
            T_val = AmplitudoL + T_shift ;
    }
    return(T_val);
}

```

```

REAL eval_time_f ;

REAL f(const REAL_D x)          /* -Delta u, not optional      */
{
    FUNCNAME("f");

    return(0.0);
}

/*****

REAL T(const REAL_D x)
{
    FUNCNAME("T"); /* Exact solution for T, optional      */
                  /* For comparison to the numerical solution,
                     * set in the driver: ANALYTIC 1
                     */
    REAL T_val, phase_pos ;
    REAL Kappa_s = k_s/c_s, Kappa_l = k_l/c_l, ratioK ;
    REAL erfPhi = erf(phi_root), erfcPhi;
    REAL sqrt_1S, sqrt_1L ;
    sqrt_1S = 0.5/sqrt(Kappa_s*eval_time_T) ;
    sqrt_1L = 0.5/sqrt(Kappa_l*eval_time_T) ;
    ratioK = sqrt(Kappa_s/Kappa_l) ;

    erfcPhi = erfc(ratioK*phi_root) ;

    phase_pos = 2.0*phi_root*sqrt(Kappa_s*eval_time_T);
    if(eval_time_T != 0.0)
    {
        if(x[0]<=phase_pos)
            T_val = AmplitudoL*(1.0 - erf(x[0]*sqrt_1S)/erfPhi) ;
        else
            T_val = AmplitudoR*(1.0 - erfc(x[0]*sqrt_1L)/erfcPhi) ;
    }
    else
    {

```



```

        if(x[0]!=0.0)
            T_val = AmplitudoR ;
        else
            T_val = AmplitudoL ;
        }
    return(T_val);
}

REAL T0(const REAL_D x)
{
    FUNCNAME("T0"); /* initial values for T, not optional      */
    REAL T_val ;

    /* eval_time_T = 926.098 ; */
    eval_time_T = 0.098 ;

    if(x[0] <=0.5)
        T_val = AmplitudoL ;
    else
        T_val = AmplitudoR ;

    return(T_val);
}

REAL eval_time_u ;

REAL u(const REAL_D x)
{
    FUNCNAME("u");

    eval_time_T = eval_time_u ;

    return(T(x));
}

REAL eval_time_H ;
REAL eval_time_u_D ;

```

```

REAL u_D(const REAL_D x)          /* boundary values for u, not optional*/
{
    FUNCNAME("u_D");
    /* provide expression for u_D !!                                     */
    /*      g = u_D                                                    */
    REAL u_val ;

    eval_time_T_D = eval_time_u_D ;

    return(T_D(x));
}
/*****

```

Remark

In principle, the main driver program able to cater temperature dependent material parameter. This pointed out previously through a user supplied functions, i.e. called by the driver program through `UtoH` function which called by `nl sor` in the `solver()`. Within current implementation, we dealt only constant properties of material. To extends it's capability, the extension needed is: implement efficiently the functions $\beta^{-1}(u)$, which is not available in general case. One way to handled this is through an array storing Temperature (Θ), Enthalpy (H), and generalized Temperature (u), as a (dynamic) table, equiped with an efficient search function on it. This requirement is important, since during each iteration in the `nl sor`, the functions called **twice** for each vector component being iterated.

APPENDIX B.

Nonlinear SOR source Code.

We give in the following a complete source code for nonlinear SOR solver, whereonly the function r is available. In the case its derivative is available, the code is easily modified, by replacing numerical approximation of derivatives in the newton iteration of root finder by a supplied analytical derivatives. An example of the prototype routine of this case is of the following :

```
int nlsor_s(const DOF_MATRIX *a, const DOF_REAL_VEC *b, const DOF_REAL_VEC *f,
            const DOF_SCHAR_VEC *bound, REAL (*phi)(const REAL),
            REAL (*Dphi)(const REAL),
            DOF_REAL_VEC *u, REAL omega, REAL tol, int max_iter, int info)
```

The complete nonlinear SOR, where the analytical derivative is not available are provided in the next code write-up.

```
/* **** */
/* ALBERT:  an Adaptive multi Level finite element toolbox using          */
/*           Bisectioning refinement and Error control by Residual        */
/*           Techniques                                                    */
/* **** */
/* file:     nlsor.c                                                       */
/* **** */
/* **** */
/* description: Solving systems of non-linear equation of the form:      */
/*               B \phi(u) + A u = b                                     */
/*               where : B is a diagonal matrix stored as a vector        */
/*               A ia a symmetric matrix (sparse)                        */
/*               \phi(u) scalar value function of variables u            */
/*               for the algorithms see book  of White or Free and Moving Boundary */
/*               Value Problems Lecture Notes by Knabner                  */
/* **** */
/* history:  */
/* **** */
/* **** */
/* **** */
```

```

/*                                                                    */
/*      authors: Alfred Schmidt and Kunibert G. Siebert              */
/*      Institut f"ur Angewandte Mathematik                          */
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/*                                                                    */
/*      (c) by A. Schmidt and K.G. Siebert (1996-2000)              */
/*      (c) by A. D. Garnadi          (2001)                        */
/*                                                                    */
/*****                                                                    */
/*****                                                                    */
/*****                                                                    */
/*****      NONLINEAR      SOR      *****/
/*****                                                                    */
/*****                                                                    */

#include "albert.h"

int nlsor_s(const DOF_MATRIX *a, const DOF_REAL_VEC *b, const DOF_REAL_VEC *f,
            const DOF_SCHAR_VEC *bound, REAL (*phi)(const REAL),
            DOF_REAL_VEC *u, REAL omega, REAL tol, int max_iter, int info)
{
    FUNCNAME("nlsor_s");
    const REAL    *fvec;
    REAL          *uvec;
    const S_CHAR  *bvec;
    REAL          max, omega1, accu, unew;
    int           j, jcol, iter;
    MATRIX_ROW    *row_a;
    REAL          *bDiag ;

    REAL val_star, w_bar, dPhi, boundNewton = 2.0e-4, dVal, h=1.0e-3 ;

```

```

bDiag = b->vec ;
fvec = f->vec;
uvec = u->vec;
bvec = bound ? bound->vec : nil;

if (omega <= 0 \vert\vert omega > 2)
{
    ERROR("omega %le not in (0,2], setting omega = 1.0\n", omega);
    omega = 1.0;
}
omega1 = 1.0 - omega;

if (info >= 2)
    MSG("omega = %.3lf, tol = %.3le, max_iter = %d\n", omega, tol, max_iter);

for (iter = 0; iter < max_iter; iter++)
{
    max = 0.0;

    FOR_ALL_DOFS(u->fe_space->admin,
if (!bvec \vert\vert bvec[dof] < DIRICHLET)
{
    accu = 0.0;
    for (row_a = a->matrix_row[dof]; row_a; row_a = row_a->next) {
        for (j=0; j<ROW_LENGTH; j++) {
            jcol = row_a->col[j];
            if (ENTRY_USED(jcol) && (jcol != dof)) {
                accu += row_a->entry[j] * uvec[jcol];
            }
            else {
if (jcol == NO_MORE_ENTRIES)
                break;
            }
        }
    }
    if ((row_a = a->matrix_row[dof]))
{

```

```

        w_bar = (fvec[dof]-accu)    ;

    val_star = uvec[dof] ; /* initialization
        MSG("val_star initialization:",w_bar);*/
    /* Newton Step : (White, p 229)                                     */
    do{
        dVal = row_a->entry[0]*val_star ;
        dVal += bDiag[dof]*phi(val_star) - w_bar ;
        dPhi = row_a->entry[0]*(val_star + h) ;
        dPhi += bDiag[dof]*phi(val_star + h) - w_bar ;
        dPhi -= dVal ;
        dVal *= h ;
        dVal = dVal/dPhi ;
        val_star -= dVal ;

        }while(dVal > boundNewton) ;

        unew = omega1*uvec[dof] + omega*val_star ;
    }
    else
    {
        unew = 0.0;
    }
    max = MAX(max, ABS(uvec[dof] - unew));
    uvec[dof] = unew;
}

);

    if (info >= 4)
        MSG("iter %3d: max = %.3le\n",iter,max);

    if (max < tol) break;
}

if (info >= 2)
{

```

```
    if (iter < max_iter)
        MSG("convergence after iter %3d: max = %.3le\n", iter, max);
    else
        MSG("NO CONVERGENCE after iter %3d: max = %.3le\n", iter, max);
}
return(iter);
}
```