Heat Transfer with Explicit SPH Method in LS-DYNA

Jingxiao Xu
LSTC

Abstract

In this paper, we introduce an explicit formalism to model heat conduction with Smoothed Particle Hydrodynamics method. With Taylor series approximation and SPH kernel interpolation, a simpler SPH discretization of the Laplace operator can be obtained for the thermal conduction equation. The formulation manifestly conserves thermal energy and is stable in the presence of small-scale temperature noise. This formalism allows us to evolve the thermal diffusion equation with an explicit time integration scheme along with the ordinary hydrodynamics. A series of simple test problems were used to demonstrate the robustness and accuracy of the method. Heat transfer with explicit SPH method can be coupled with structure for thermal stress and thermal structure coupling analysis.

Introduction

Heat transfer is very important in many industrial and geophysical problems. Many of the problems of geophysical and industrial fluid dynamics involve complex flows of multiple liquids and gases coupled with heat transfer. The motion of the surfaces of the liquids can involve sloshing, splashing and fragmentation. Thermal and chemical processes present further complications. The simulation of such systems can sometimes present difficulties for finite difference and finite element methods, particularly when coupled with complex free surface motion, while smoothed particle hydrodynamics can easily follow wave breaking, and it provides a reasonable simulation of splash on a length scale exceeding that where surface tension must be included.

SPH is a Lagrangian method for solving partial differential equations. Essentially, the domain is discretized by approximating it by a series of roughly equi-spaced particles. They move and change their properties (such as temperature) in accordance with a set of ordinary differential equations derived from the original governing PDEs. SPH was first applied by Lucy (1977) to astrophysical problems, and was extended by Gingold (1982). Cloutman (1991) used SPH to model hypervelocity impacts. Libersky and Petschk have shown that SPH can be used to model materials with strength. In recent years it has been developed as a method for incompressible isothermal enclosed flows by Monaghan (1994).

Cleary and Monaghan (1995) extended the method to heat conduction and then to coupled heat and mass flows due to that SPH has a range of strong advantages in modeling industrial heat and mass flows:

1. The Lagrangian framework allows momentum dominated flows to be easily handled.
2. Complex free surface and material interface behavior, including break-up into fragments, can be modeled naturally.
3. Complicated physics such as multi-phase, realistic equations of state, compressibility, radiation, solidification and fracturing can be added with comparative ease.
4. Is easily extendible to three dimensions.

M. Jubelgas, V. Springel and K. Dolag (2004) introduced a new formalism to model conduction in a diffuse ionized plasma using smoothed particle hydrodynamics, they considered only isotropic conduction and assumed that magnetic suppression can be described in terms of an effective conductivity. An explicit time integration scheme along with ordinary hydrodynamics was used to evolve the thermal diffusion equation, and the results showed the accuracy and robustness of the method.

In this paper, we introduced an explicit formalism to model heat conduction with Smoothed Particle Hydrodynamics method in the LS-DYNA code. With Taylor series approximation and SPH kernel interpolation, a simpler SPH discretization of the Laplace operator can be obtained for the thermal conduction equation. The formulation manifestly conserves thermal energy and is stable in the presence of small-scale temperature noise. This formalism allows us to evolve the thermal diffusion equation with an explicit time integration scheme along with the ordinary hydrodynamics.

Thermal conduction in SPH

Fundamentals of the SPH method.

Particles methods are based on quadrature formulas on moving particles $(x_i(t), w_i(t)) i \in P$, P is the set of the particles. $x_i(t)$ is the location of particle i and $w_i(t)$ is the weight of the particle i. The quadrature formulation for a function can be written as:

$$\int_{\Omega} f(x)dx = \sum_{j \in P} w_j(t) f(x_j(t)) \tag{1}$$

The quadrature formulation (1) together with the definition of smoothing kernel leads to the definition of the particle approximation of a function. The interpolated value of a function: $u(X)$ at position X using the SPH method is:

$$\prod^h (u(x_i)) = \sum_{j \in \Omega} w_j(t) u(x_j) W(x_i - x_j, h) \tag{2}$$

Where the sum is over all particles inside Ω and within a radius $2h$, W is a spline based interpolation kernel of radius $2h$. It mimics the shape of a delta function but without the infinite tails. It is a C^2 function. The kernel function is defined as following:

$$W(x_i - x_j, h) = \frac{1}{h} \theta \left\{ \frac{x_i - x_j}{h(x, y)} \right\} \tag{3}$$

$W(x_i - x_j, h) \to \delta$ when $h \to 0$, δ is Dirac function, h is a function of x_i and x_j and is the so-called smoothing length of the kernel.

And the cubic B-spline function is defined:

$$\theta(d) = C \times \begin{cases} 1 - \frac{3}{2}d^2 + \frac{3}{4}d^3 & \text{when } 0 \le d \le 1 \\ \frac{1}{4}(2-d)^3 & \text{when } 1 \le d \le 2 \\ 0 & \text{elsewhere} \end{cases} \tag{4}$$

The gradient of the function $u(X)$ is given by applying the operator of derivation on the smoothing length:

$$\nabla \prod^h (u(x_i) = \sum_j w_j u(x_j) \nabla W(x_i - x_j, h) \tag{5}$$

Evaluating an interpolated product of two functions is given by the product of their interpolated values.

Continuity equation and Momentum equation.

The particle approximation of continuity equation is defined as:

$$\frac{d\rho_i}{dt} = \rho_i \sum_j \frac{m_j}{\rho_j} \left(v^{\beta}{}_i - v^{\beta}{}_j \right) W_{ij'\beta} \tag{6}$$

It is Galilean invariant due to that the positions and velocities appear only as differences, and has good numerical conservation properties. $v^{\beta}{}_i$ is the velocity component at particle i.

The discretized form of the SPH momentum equation is developed as:

$$\frac{dv_i^{\alpha}}{dt} = -\sum_j \frac{m_j}{\rho_i \rho_j} (\sigma_i^{\alpha\beta} \pm \sigma_j^{\alpha\beta}) W_{ij,\beta} \tag{7}$$

The above formulation ensures that stress is automatically continuous across material interfaces. Different types of SPH momentum equations can be achieved through applying the identity equations into the normal SPH momentum equation. Symmetric formulation of SPH momentum equation can reduce the errors arising from particle inconsistency problem.

Conduction equation for SPH.

Heat conduction is a transport process for thermal energy, driven by temperature gradients in the conduction medium. Define the local heat flux as:

$$j = -\kappa \nabla T \tag{8}$$

Where T gives the temperature field, and κ is the heat conduction coefficient, which may depend on local properties of the medium.

The rate of temperature change induced by conduction can simply be obtained from conservation of energy:

$$\frac{du}{dt} = \frac{1}{\rho} \nabla \cdot (\kappa \nabla T) \tag{9}$$

Where u is the thermal energy per unit mass, temperature is typically simply proportional to u, unless the mean particle weight changes in the relevant temperature regime. For all practical purposes: $u = c_v T$, c_v is the heat capacity per unit mass.

A simple discretization of the conduction equation in SPH can be obtained by first estimating the heat flux for each particle applying standard kernel interpolation method, then estimating the divergence in a second step. However, this method has been shown to be quite sensitive to particle disorder, which can be traced to the effective double-differentiation of the SPH-kernel. It is hence advantageous to use a simpler SPH discretization of the Laplace operator, which should ideally involve only first order derivatives of the smoothing kernel (Brookshaw 1985, Martin Jubelgas 2004).

For a well-behaved field $Y(x)$, begin with a Taylor-series approximation, neglect terms of third and higher orders and multiply with the SPH smoothing kernel function, a discrete SPH approximation of the Laplace operator can deduced:

$$\nabla^2 Y \Big|_i = -2 \sum_j \frac{m_j}{\rho_j} \frac{Y_j - Y_i}{\left| x^2{}_{ij} \right|} x_{ij} \nabla_i W_{ij} \tag{10}$$

By applying a discrete SPH approximation of the Laplace operator to the thermal conduction problem, a simpler discretized form of equation (9) can be obtained:

$$\frac{du_i}{dt} = \sum_j \frac{m_j}{\rho_i \rho_j} \frac{(\kappa_i - \kappa_j)(T_j - T_i)}{\left| x_{ij} \right|^2} x_{ij} \nabla_i W_{ij} \tag{11}$$

This form is antisymmetric in the particles i and j, and the energy exchange is always balanced on a pairwise basis.

The maximum time step for the explicit integration of the energy equation is:

$$\Delta t = \varsigma \rho c_v h^2 / \kappa \tag{12}$$

Detailed stability tests were performed for a range of material parameters and showed that

$\varsigma = 0.1$ was sufficient to guarantee stability.

Thermal initial condition and boundary condition.

The default thermal boundary condition is adiabatic. Any SPH particle on a surface is effectively adiabatic, since they are no particles beyond with which they can exchange energy. This is an automatic natural boundary condition.

Initial temperature condition can be applied to the SPH particles through keyword: *INITIAL_TEMPEARTURE_OPTION. Thermal boundary condition for SPH particles can be realized through keyword: *BOUNDARY_TEMPERATURE_OPTION. These two thermal conditions will be applied on the SPH particles directly.

Flux boundary condition can be applied to the surface segments (defined by a set of segments from SPH particles) through keyword: BONDARY_FLUX_OPTION. Heat flow is negative in the direction of surface normal vector (left hand rule as shown in the Fig. 1).

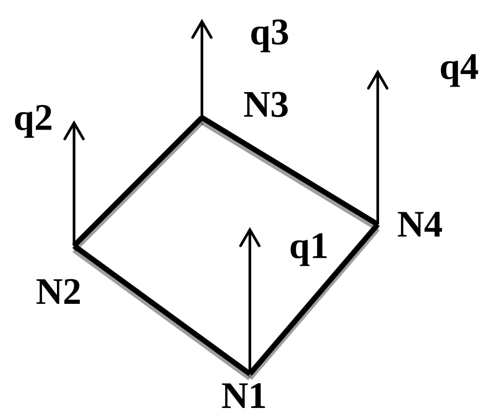

Fig. 1. Heat flow direction

Keyword in LS-DYNA for thermal SPH

The thermal option for SPH can be activated by setting SOLN=2 in *CONTROL_SOLUTION card. The parameter Eqheat (mechanical equivalent of heat conversion factor) and fwork (fraction of mechanical work converted in to heat) in *CONTROL_THERMAL_SOLVER card can be used for coupling thermal structure analysis:

$$(eqheat)(fwork)w = \rho c \Delta T \tag{13}$$

Thermal material property identification (TMID in *PART card) defined in the *MAT_THERMAL keyword has to be specified for the thermal option of SPH. *MAT_VISCOELASTIC_THERMAL model can be used for SPH particles to apply the thermal stresses, more material models with thermal stresses will be added for SPH particles. *MAT_ADD_THERMAL_EXPANSION was supported for the SPH particles and was used to occupy an arbitrary material model supported by SPH with a thermal expansion property.

Examples

1. 3D heat conduction problem.

3D heat conduction model with dimension of 0.1 by 0.1 and length of 1.0 was calculated to demonstrate the accuracy and robustness of the SPH explicit thermal solver in LS-DYNA. The problem was modeled with both solid elements and SPH particles. For both parts, initial temperature was set to 0.0, a temperature boundary condition of 1.0 was set on surface nodes of the left hand side and an adiabatic thermal boundary condition for all other surfaces was set, a plastic-kinematic structure material model with ISOTROPIC thermal material property was used. For solid elements, an implicit thermal solver (iterative conjugated gradient method) was used, while the explicit thermal solver was used for SPH.

Comparing the time steps, SPH required time step to be 6.25E-5 (which was more than 1000 times smaller than the time step of solid elements) while the time step for solid elements was: 2.00E-1 due to that SPH particles used explicit thermal solver and solid elements used implicit thermal solver. Temperature results from SPH particles are comparable with results from solid elements (Fig. 3). The nodal temperature history for the solid node and SPH particle at the same location of the horizontal axis were plotted and compared in Fig.4, two results were very close.

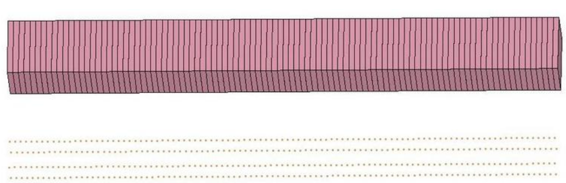

Fig. 2. Problem set up (apply temperature at left side)

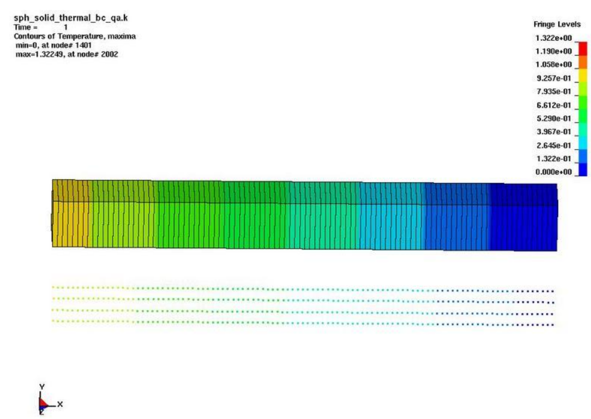

Fig. 3. Final temperature contour plot

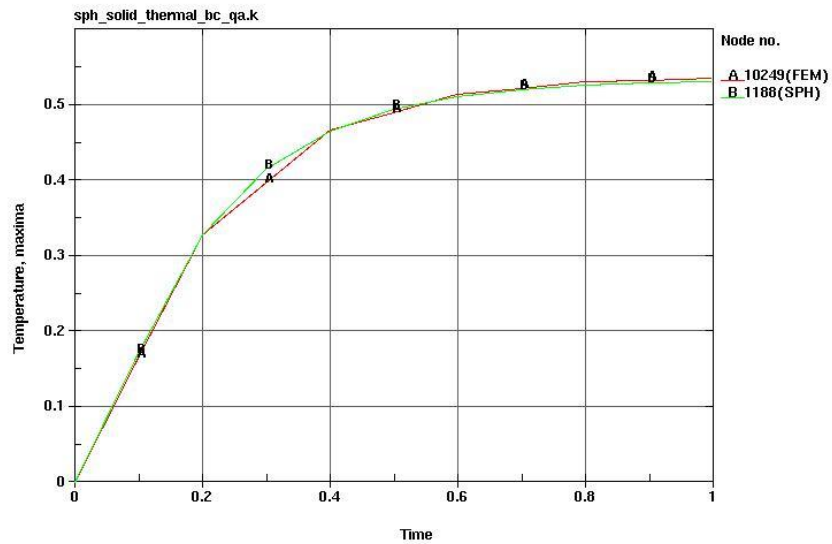

Fig. 4. Nodal temperature history plot for solid node and SPH particle at the same location of horizontal axis.

Next, the same setup was used, but the heat flux temperature boundary conditions were applied on the segments of the left hand side of both parts and adiabatic thermal boundary conditions for all other surfaces. The heat source is described by heat flux q: W/mm2. To compare the results from solid elements with the results from the SPH particles, the Heat_flux*Area for segments from solid element and segments generated from SPH particle needed to be the same. Four SPH particles on the left hand side formed a segment for flux boundary condition. The nodal temperature history for the solid node and SPH particle at the same location of the horizontal axis are plotted and compared in Fig.5, two results were very close.

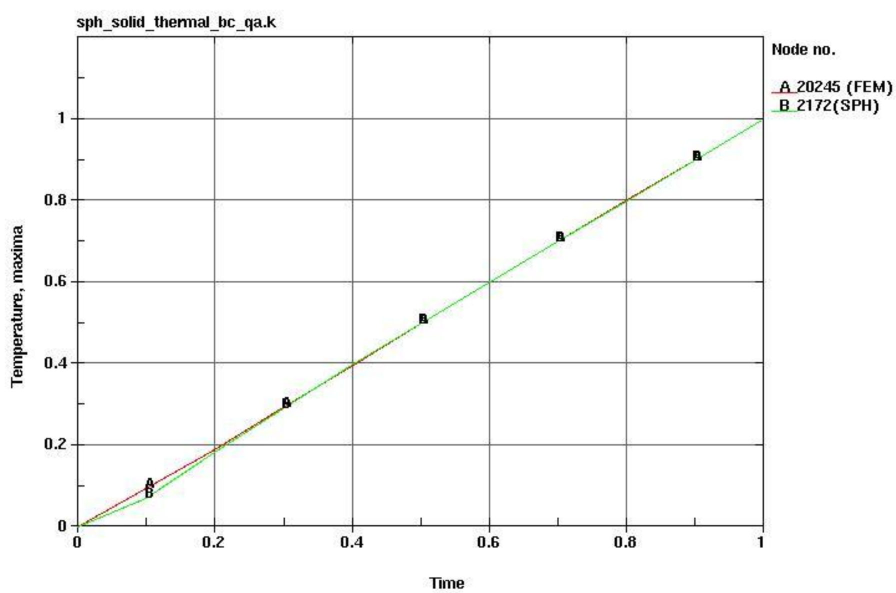

Fig. 5. Nodal temperature history plot for solid node and SPH particle at the same location of horizontal axis.

2. Thermal expansion testing.

A simple example was modeled with solid elements and SPH particles with crushable foam material and ISOTROPIC thermal properties as shown in Fig. 6. Adiabatic thermal boundary conditions were applied on all surfaces of the model. These two parts were loaded uniformly throughout the model with the temperature through *LOAD_THERMAL_LOAD_CURVE keyword. The temperatures of both parts were raised linearly with respect to time. *MAT_ADD_THERMAL_EXPANSION was added for both parts with expansion scale factor=0.5 to account for the expansion due to thermal. As shown in Fig. 7, both parts were expanded properly due to the change of the temperatures. Results from SPH particles were comparable to the results from solid elements.

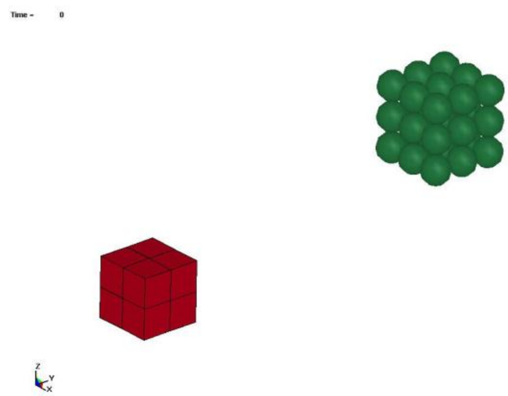

Fig. 6. Solid elements and SPH particles before expansion.

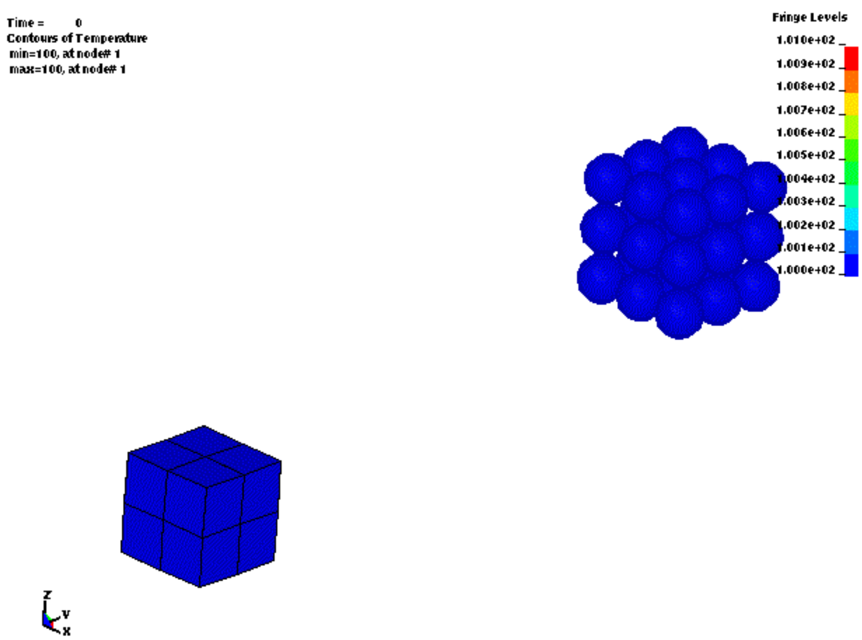

Fig. 7. Solid elements and SPH particles after expansion.

The distance of the diagonal length on the top surface were measured and compared. The original distance of the diagonal length for both parts was: 1.414 before the expansion. After the expansion, the distance of the diagonal length for solid elements was: 2.015 and the distance of the diagonal length for the SPH particles was: 2.017. Two distances were almost the same.

3. SPH structure coupling with thermal.

In this example, the model with Johson_Cook material and ISOTROPIC thermal properties for the SPH particles was tested. The Taylor bar moved down with an initial speed V and contacted with rigid shell at the bottom. The temperature of the body changed due to the conversion of mechanical work into heat through plastic deformation: $(eqheat)(fwork)w = \rho c \Delta T$. The process was fast enough such that there is no heat transfer with the environment. The model had initial temperature of 0 degree, and the increase of the temperature of the Taylor bar was completely due to the conversion of plastic work to heat. Fig.9 and Fig.10 showed the plastic contour plot and the temperature contour (due to plastic deformation) plot after the conversion.

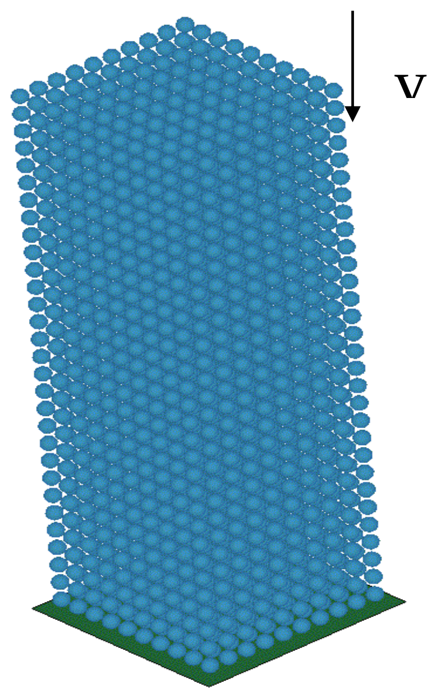

Fig. 8. Taylor bar set up.

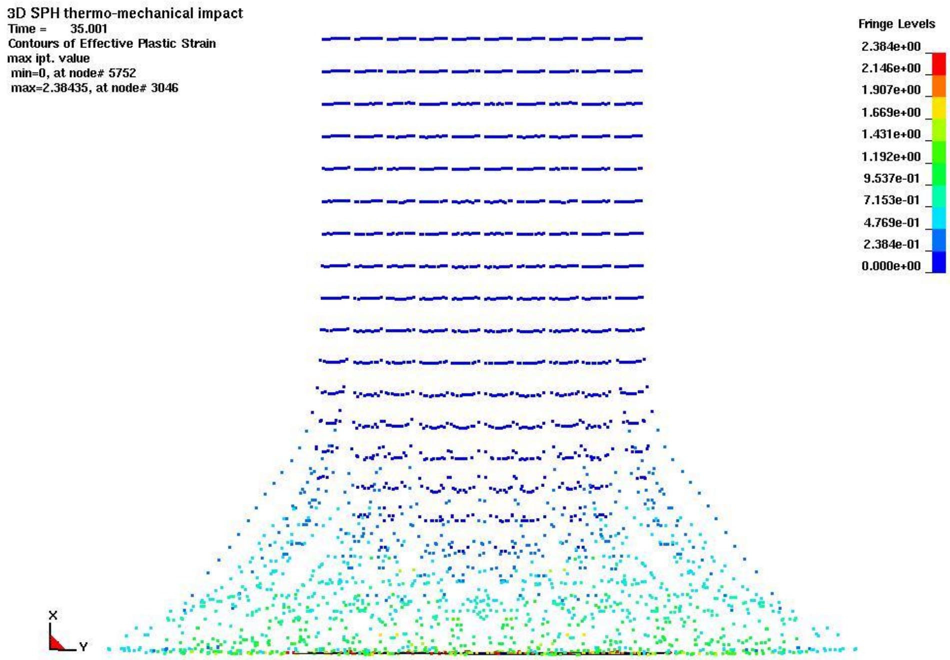

Fig. 9. Effective plastic strain contour plot for Taylor bar.

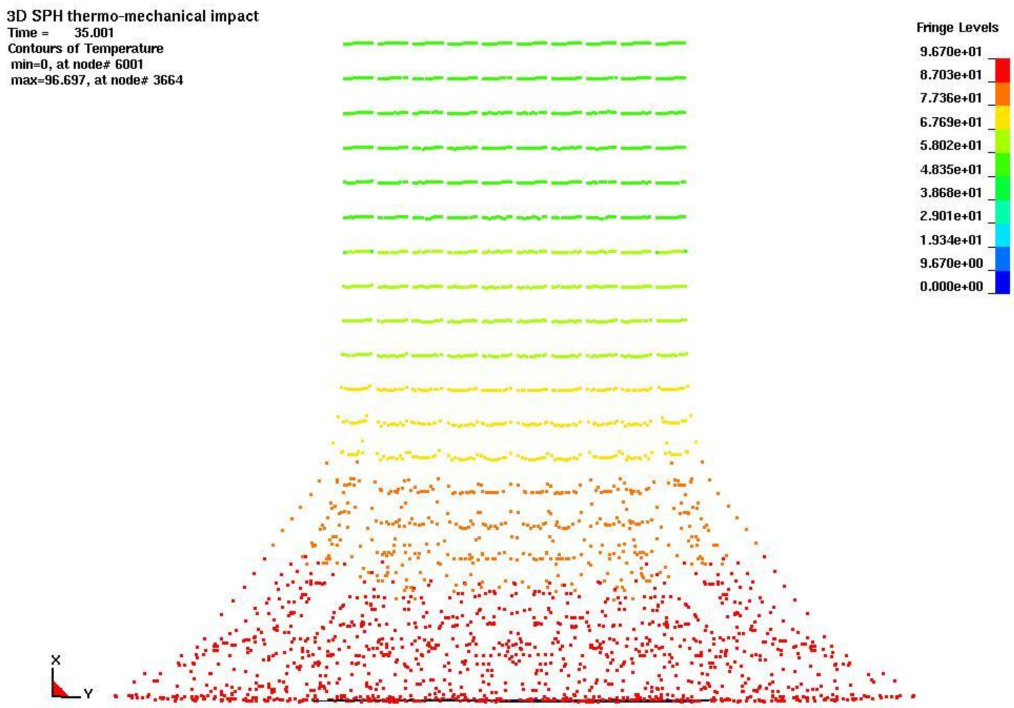

Fig. 10. Temperature contour plot for Taylor bar.

CONCLUSION

An explicit formalism for heat conduction with Smoothed Particle Hydrodynamics method was developed in LS-DYNA code. A series of simple test problems were used to demonstrate the capabilities of LS-DYNA in thermal option with SPH particles. Heat transfer with explicit SPH method can be coupled with structure for thermal stress and thermal structure coupling analysis. New features under development include:

1. More thermal BCs for SPH: Boundary_convection, Boundary_radiation and so on.
2. More thermal stress material models for SPH particles.
3. Possibly a new algorithm of thermal contact between SPH particles and solid elements and shell elements needs to be developed.

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