

A COMPLETE TREATMENT OF THERMO-MECHANICAL ALE ANALYSIS; PART I: FORMULATION*

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Abstract– Arbitrary Lagrangian Eulerian (ALE) finite element method is extensively used for numerical simulation of solid mechanics problem. The versatility of the mesh in ALE approach makes it particularly effective and efficient in solving large deformation problems. In this work, a complete treatment of fully coupled ALE formulation is presented incorporating inertial, rate and thermal effects. The formulation may be used in conjunction with thermo-elasto-viscoplastic material models. A consistent and efficient tangent operator is developed in closed form to handle stress integration. The applications of this formulation are given in the second part of this paper.

Keywords– Arbitrary Lagrangian Eulerian, finite element method, large deformation, implicit dynamic analysis, thermo-mechanical, viscoplastic

1. INTRODUCTION

Finite element method has been extensively used for numerical simulation of large deformation problems such as analysis of metal forming applications. From the numerical viewpoint, two main approaches have been traditionally used for large deformation simulations; the Lagrangian approach and the Eulerian approach. In the Lagrangian approach, commonly used for simulation of solid mechanics problems, the finite element mesh is attached to the material and follows its deformation. As a result, the mesh will undergo severe mesh distortion when large deformation occurs, requiring frequent remeshing. In the Eulerian approach, on the other hand, the mesh is fixed in space and the material flows through it. Therefore, the Eulerian approach is a natural approach for simulation of fluid flow problems, where the boundaries of deformation are known in advance. However, this approach is inefficient in simulation of development of material free boundaries during deformation. To avoid the shortcomings of the above two approaches, a third and more general approach known as Arbitrary Lagrangian-Eulerian method (ALE) is developed, combining the advantages of both the Lagrangian and Eulerian approaches while avoiding their shortcomings. In an ALE analysis, the FE mesh is neither attached to the material nor fixed in space, but can have any arbitrary, user-defined motion independent of the material. The use of this method has gained popularity in recent years and in many applications [1-6]. However, development of a consistent ALE formulation and the design of proper mesh motion are challenging tasks, and have given rise to various forms of ALE approach in the literature. The migration of material points through the grid which is inherent to the ALE analysis, gives rise to convective terms relating the material time derivative to the grid time derivatives. From the point of view of handling the convective terms, the ALE formulations in the literature are divided into coupled formulation [5, 10-17] and operator-split formulation [7-9]. The former approach solves the material motion and convection steps simultaneously, whereas the latter

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approach divides the solution into a Lagrangian step followed by a convection step. The obvious advantage of the operator-split approach is in its simplicity and computational convenience, but it is, in effect, equivalent to an updated Lagrangian formulation combined with consecutive remeshing. In contrast, the coupled solution represents the true description of equilibrium at each step.

In this paper, a systematic derivation of the fully coupled dynamic ALE formulation based on ALE forms of equation of motion and energy equation that is suitable for application to thermo-mechanical analysis of large deformation solid mechanics problems is presented. Starting from the principle of virtual work and thermodynamic equilibrium, ALE equations are developed. The treatment of a viscoplastic material model based on the consistency model [18] is presented and a new consistent tangent operator in closed form is developed to handle stress updating. The differences between the presented formulation and previous works in the literature are discussed. In the second part of this paper, the finite element form of the ALE equations will be derived and the numerical simulations of a few example problems will be presented.

2. CONSERVATION LAWS OF THE CONTINUA

a) Kinematics

In the ALE analysis, the finite element grid points are allowed to have an arbitrary motion independent of material motion that happens as a result of deformation under given loads. Therefore, three frames of reference are used to describe the material deformation; the material, the spatial and the referential frames [12]. Due to the independence of the material and grid motions, two sets of velocities are needed to determine the motion, the velocity of a material point ${}^t v_i$ and the velocity of a grid point ${}^t v_i^g$, with the latter being expressed in terms of referential frame. Though these velocities are, in general, independent of each other, there should exist a one-to-one mapping between the two, i.e., at any given time, each grid point should coincide with one and only one material point. Furthermore, the difference between the two velocities is defined as the convective velocity ${}^t c_i$. The mapping between the two descriptions should be in a way that the boundaries of the material and grid domains coincide, i.e.,

$$({}^t v_i - {}^t v_i^g) {}^t n_i |_S = 0 \quad (1)$$

where S is the domain boundary, ${}^t n_i$ is the unit normal vector at any point on the boundary, and the left superscript describes the time at which the quantity is measured. In the ALE conservation laws of the continua, the relationship between the material time rate and the grid time rate of an arbitrary function $f(x,t)$ must be defined. In the ALE description, the fundamental relation between material time derivatives, grid time derivatives, and the spatial gradient of $f(x,t)$ is given as [4]

$${}^t \dot{f} = {}^t f' + {}^t c_i \frac{\partial {}^t f}{\partial {}^t x_i} = {}^t f' + ({}^t v_i - {}^t v_i^g) \frac{\partial {}^t f}{\partial {}^t x_i} \quad (2)$$

where ${}^t f'$ and ${}^t \dot{f}$ are grid and material time derivatives, respectively.

b) Conservation of mass

The strong form of conservation law for mass in the spatial coordinate system at time t is given by

$${}^t \dot{\rho} = -{}^t \rho \frac{\partial {}^t v_i}{\partial {}^t x_i} \quad (3)$$

where ${}^t\rho$ is the material density. Using (2), the ALE form of Eq. (3) can be expressed with respect to the referential frame as

$${}^t\rho' = -{}^t\rho \frac{\partial {}^t v_i}{\partial {}^t x_i} - {}^t c_i \frac{\partial {}^t \rho}{\partial {}^t x_i} \quad (4)$$

c) Conservation of momentum

The equation of motion in the ALE analysis can be derived from the law of conservation of momentum. Using the principle of virtual work, the weak form of this law expressing the balance of momentum at time $t + \Delta t$ can be given as [5]

$$\int_{t+\Delta t V} {}^{t+\Delta t} \sigma_{ij} \frac{\partial \delta u_i}{\partial {}^{t+\Delta t} x_j} {}^{t+\Delta t} dV + \int_{t+\Delta t V} {}^{t+\Delta t} \rho {}^{t+\Delta t} \dot{v}_i \delta u_i {}^{t+\Delta t} dV = \int_{t+\Delta t V} {}^{t+\Delta t} \rho {}^{t+\Delta t} f_i^B \delta u_i {}^{t+\Delta t} dV + \int_{t+\Delta t A} {}^{t+\Delta t} f_i^S \delta u_i {}^{t+\Delta t} dA \quad (5)$$

where ${}^{t+\Delta t} \sigma_{ij}$ are the components of the Cauchy stress tensor at time $t + \Delta t$, and ${}^{t+\Delta t} f_i^B$ are the components of the body force per unit mass at time $t + \Delta t$.

d) Conservation of energy

In deformation processes involving significant conversion of mechanical energy to heat, the law of conservation of energy should be satisfied to uphold the thermodynamic equilibrium. The balance of energy is expressed as [19, 20]

$$\rho c_p \dot{T} = \dot{W}^{irr} + \rho r - q_{i,i} \quad (6)$$

where c_p is the specific heat, T is temperature, r is the internal heat source, q_i is the thermal flux in direction i and \dot{W}^{irr} is the dissipation term expressed as

$$\dot{W}^{irr} = \chi \bar{\sigma} \dot{\bar{\epsilon}}^p \quad (7)$$

where χ is the Taylor-Quinney factor [21] expressing the portion of plastic energy converted to heat, commonly between 0.85 and 0.95, $\bar{\sigma}$ is the equivalent stress and $\dot{\bar{\epsilon}}^p$ is the effective plastic strain rate. Using the Fourier's law for general medium written as $q_i = -k_{ij} T_{,j}$ where k_{ij} is the conductivity coefficients, Eq. (6) can be written as

$$\rho c_p \dot{T} = \dot{W}^{irr} + \rho r + (k_{ij} T_{,j})_{,i} \quad (8)$$

The boundary conditions for thermal problems (excluding radiation) are expressed as

$$q_i n_i = -q_s |_{S_1} + h(T_s - T_\infty) |_{S_2} \quad \text{and} \quad T |_{S_3} = T_s \quad (9)$$

representing specified flux, convection and specified temperature on respective parts of the boundary, S_1 to S_3 . Here, h is the convection coefficient and \mathbf{n} is the surface normal vector. By applying the divergence theorem to the third term on the right-hand side of Eq. (8) to include boundary conditions, the weak form of equation of balance of energy at time $t + \Delta t$ may be described as

$$\begin{aligned} & \int_{t+\Delta t V} \delta T {}^{t+\Delta t} c_p {}^{t+\Delta t} \dot{T} {}^{t+\Delta t} \rho {}^{t+\Delta t} dV + \int_{t+\Delta t V} \frac{\partial \delta T}{\partial {}^{t+\Delta t} x_i} {}^{t+\Delta t} k_{ij} \frac{\partial {}^{t+\Delta t} T}{\partial {}^{t+\Delta t} x_j} {}^{t+\Delta t} dV = \\ & \int_{t+\Delta t V} \delta T {}^{t+\Delta t} \rho {}^{t+\Delta t} r {}^{t+\Delta t} dV + \int_{t+\Delta t V} \delta T {}^{t+\Delta t} \dot{W}^{irr} {}^{t+\Delta t} dV - \\ & \int_{t+\Delta t S} \delta T {}^{t+\Delta t} q_i {}^{t+\Delta t} n_i {}^{t+\Delta t} dS \end{aligned} \quad (10)$$

3. INCREMENTAL FORM OF CONSERVATION LAWS

a) Incremental decomposition of variables

Starting from Eq. (5) and referring all variables at time $t + \Delta t$ to the grid configuration at time t , the variables can be decomposed into their value at time t plus an increment written in terms of their time derivative with respect to the grid. In this way, the material density at time $t + \Delta t$ is expressed as

$${}^{t+\Delta t}\rho = {}^t\rho + {}^t\rho'\Delta t \quad (11)$$

Substituting (4) into (11) gives

$${}^{t+\Delta t}\rho = {}^t\rho - \left({}^t\rho \frac{\partial {}^t v_k}{\partial {}^t x_k} + {}^t c_k \frac{\partial {}^t \rho}{\partial {}^t x_k} \right) \Delta t \quad (12)$$

Similarly, the stress components can be decomposed into an incremental form;

$${}^{t+\Delta t}\sigma_{ij} = {}^t\sigma_{ij} + {}^t\dot{\sigma}_{ij}\Delta t - (u_k - u_k^g) \frac{\partial {}^t\sigma_{ij}}{\partial {}^t x_k} \quad (13)$$

where ${}^t\dot{\sigma}_{ij}$ is the material time derivative of Cauchy stress. The volume element at time $t + \Delta t$ is related to the volume element at time t through the following equation [5]

$${}^{t+\Delta t}dV = {}^tdV + \frac{\partial u_k^g}{\partial {}^t x_k} {}^tdV \quad (14)$$

Similarly, elemental surface area ($dA_j = n_j dS$) at time $t + \Delta t$ is related to elemental area at time t through the following equation [5]

$${}^{t+\Delta t}(dA) = {}^tdA + \left[\frac{\partial u_k^g}{\partial {}^t x_k} - \frac{1}{2} {}^t n_m \left(\frac{\partial u_m^g}{\partial {}^t x_n} + \frac{\partial u_n^g}{\partial {}^t x_m} \right) {}^t n_n \right] {}^tdA \quad (15)$$

Furthermore, the spatial derivatives of a function $f(x, t)$ with respect to the spatial coordinate at time $t + \Delta t$ may be expressed with respect to the spatial coordinate at time t as follows

$$\frac{\partial {}^t f}{\partial {}^{t+\Delta t} x_j} = \frac{\partial {}^t f}{\partial {}^t x_j} - \frac{\partial {}^t f_i}{\partial {}^t x_k} \frac{\partial {}^t v_k^g}{\partial {}^t x_j} \Delta t \quad (16)$$

Finally, the incremental decomposition of temperature in the ALE description may be expressed as

$${}^{t+\Delta t}T^i = {}^{t+\Delta t}T'^i + {}^{t+\Delta t}c_j \frac{\partial {}^{t+\Delta t}T}{\partial {}^{t+\Delta t}x_j} \quad (17)$$

b) Incremental form of equation of motion

In this section, the governing equation of motion expressed at time $t + \Delta t$ is linearized by decomposing it into incremental form. This is achieved by substituting Eqs. (12), (13), (14) and (15) into Eq. (5), and neglecting higher order differential terms. For simplicity, we treat the right (RHS) and left hand sides (LHS) of Eq. (5) separately, and then combine the two parts. Starting from the RHS, the incremental decomposition of ${}^{t+\Delta t}f_i^B$ and ${}^{t+\Delta t}f_i^S$ are written as

$${}^{t+\Delta t}f_i^B = {}^t f_i^B + f_i^B \quad \text{and} \quad {}^{t+\Delta t}f_i^S = {}^t f_i^S + f_i^S \quad (18)$$

Substituting from Eqs. (12), (14), (15) and (18) into the RHS of Eq. (5), and neglecting the higher order terms, the linearized form of RHS is obtained as:

$$\int_V \delta u_i ({}^t f_i^B + f_i^B) {}^t \rho {}^t dV - \int_V \delta u_i ({}^t f_i^B + f_i^B) \frac{\partial [{}^t \rho (u_m - u_m^g)]}{\partial {}^t x_k} {}^t dV + \int_A \delta u_i ({}^t f_i^s + f_i^s) {}^t dA + \int_A \delta u_i {}^t f_i^s \left[\frac{\partial u_k^g}{\partial {}^t x_k} - \frac{1}{2} {}^t n_m \left(\frac{\partial u_m^g}{\partial {}^t x_n} + \frac{\partial u_n^g}{\partial {}^t x_m} \right) {}^t n_n \right] {}^t dA \quad (19)$$

Substituting from Eqs. (13), (14) and (16) into the first term on the LHS of Eq. (5) and neglecting the higher order terms, this term is expressed as

$$\int_V {}^t \sigma_{ij} \frac{\partial \delta u_i}{\partial {}^t x_j} {}^t dV + \int_V \frac{\partial \delta u_i}{\partial {}^t x_j} ({}^t \dot{\sigma}_{ij} \Delta t - {}^t \sigma_{ik} \frac{\partial u_j^g}{\partial {}^t x_k} + {}^t \sigma_{ij} \frac{\partial u_k^g}{\partial {}^t x_k} - (u_k - u_k^g) \frac{\partial {}^t \sigma_{ij}}{\partial {}^t x_k}) {}^t dV \quad (20)$$

Similarly, the second term of the LHS of Eq. (5) which includes the inertial terms can be derived in a lengthy but straightforward linearization procedure as [12]:

$$\int_V \delta u_i {}^{t+\Delta t} v_i {}^t \rho {}^t dV + \int_V \delta u_i {}^t c_j \frac{\partial {}^{t+\Delta t} v_i}{\partial {}^t x_j} {}^t \rho {}^t dV - \int_V \delta u_i {}^t v_i \frac{\partial ({}^t \rho {}^t c_k)}{\partial {}^t x_k} {}^t dV \Delta t - \int_V \delta u_i {}^t c_j \frac{\partial {}^t v_i}{\partial {}^t x_j} \frac{\partial ({}^t \rho {}^t c_k)}{\partial {}^t x_k} {}^t dV \Delta t + \int_V \delta u_i {}^t c_j \frac{\partial {}^t v_i}{\partial {}^t x_j} {}^t \rho {}^t dV \Delta t - \int_V \delta u_i {}^t c_j \frac{\partial {}^t v_i}{\partial {}^t x_k} \frac{\partial {}^t v_k^g}{\partial {}^t x_j} {}^t \rho {}^t dV \Delta t \quad (21)$$

Equations (19), (20) and (21) are combined to yield the final form of ALE equation of motion, expressed in terms of variables at time t

$$\int_V \frac{\partial \delta u_i}{\partial {}^t x_j} ({}^t \dot{\sigma}_{ij} \Delta t - {}^t \sigma_{ik} \frac{\partial u_j^g}{\partial {}^t x_k} + {}^t \sigma_{ij} \frac{\partial u_k^g}{\partial {}^t x_k} - (u_k - u_k^g) \frac{\partial {}^t \sigma_{ij}}{\partial {}^t x_k}) {}^t dV + \int_V \delta u_i {}^{t+\Delta t} v_i {}^t \rho {}^t dV + \int_V \delta u_i {}^t c_j \frac{\partial {}^{t+\Delta t} v_i}{\partial {}^t x_j} {}^t \rho {}^t dV = \delta^{t+\Delta t} w^{ext} - \int_V {}^t \sigma_{ij} \frac{\partial \delta u_i}{\partial {}^t x_j} {}^t dV + \int_V \delta u_i {}^t v_i \frac{\partial ({}^t \rho {}^t c_k)}{\partial {}^t x_k} {}^t dV \Delta t + \int_V \delta u_i {}^t c_j \frac{\partial {}^t v_i}{\partial {}^t x_j} \frac{\partial ({}^t \rho {}^t c_k)}{\partial {}^t x_k} {}^t dV \Delta t - \int_V \delta u_i {}^t c_j \frac{\partial {}^t v_i}{\partial {}^t x_j} {}^t \rho {}^t dV \Delta t + \int_V \delta u_i {}^t c_j \frac{\partial {}^t v_i}{\partial {}^t x_k} \frac{\partial {}^t v_k^g}{\partial {}^t x_j} {}^t \rho {}^t dV \Delta t \quad (22)$$

where

$$\delta^{t+\Delta t} w^{ext} = \int_V \delta u_i ({}^t f_i^B + f_i^B) {}^t \rho {}^t dV - \int_V \delta u_i ({}^t f_i^B + f_i^B) \frac{\partial [{}^t \rho (u_k - u_k^g)]}{\partial {}^t x_k} {}^t dV + \int_A \delta u_i ({}^t f_i^s + f_i^s) {}^t dA + \int_A \delta u_i {}^t f_i^s \left[\frac{\partial u_k^g}{\partial {}^t x_k} - \frac{1}{2} {}^t n_m \left(\frac{\partial u_m^g}{\partial {}^t x_n} + \frac{\partial u_n^g}{\partial {}^t x_m} \right) {}^t n_n \right] {}^t dA \quad (23)$$

It is noted that the presented formulation satisfies the consistency requirement of any ALE formulation that should reduce to updated Lagrangian and Eulerian formulations as special cases under proper mesh motion conditions. If the mesh velocity is set equal to the material velocity, the formulation reduces into updated Lagrangian formulation. To show this, set ${}^t v_i = {}^t v_i^g$ or ${}^t c_i = 0$ and $(\)' = (\)$ everywhere in ${}^t V$ and on ${}^t A$ in Eq. (22) to get:

$$\int_V \frac{\partial \delta u_i}{\partial {}^t x_j} [({}^t \dot{\sigma}_{ij} - {}^t \sigma_{ik} \frac{\partial u_j}{\partial {}^t x_k}) + {}^t \sigma_{ij} \frac{\partial u_k}{\partial {}^t x_k}] {}^t dV + \int_V \delta u_i \dot{v}_i {}^t \rho {}^t dV = \int_V \delta u_i f_i^B {}^t \rho {}^t dV + \int_A \delta u_i f_i^s {}^t dA + \int_A \delta u_i {}^t f_i^s \left[\frac{\partial u_k}{\partial {}^t x_k} - \frac{1}{2} {}^t n_m \left(\frac{\partial u_m}{\partial {}^t x_n} + \frac{\partial u_n}{\partial {}^t x_m} \right) {}^t n_n \right] {}^t dA \quad (24)$$

Equation (24) is identical to the updated Lagrangian formulation in static analysis derived by McMeeking [22] except for the following correction term

$$\int_{\text{t}_A} \delta u_i f_i^s \left[\frac{\partial u_k}{\partial \text{t}_x^k} - \frac{1}{2} \text{t}_n \left(\frac{\partial u_m}{\partial \text{t}_x^m} + \frac{\partial u_n}{\partial \text{t}_x^m} \right) \text{t}_n \right] \text{t}_A dA \quad (25)$$

On the other hand, if the grid velocity is set to zero, the formulation reduces to Eulerian formulation. This can be shown by setting $\text{t}_v_i^g = 0$ or $\text{t}_c_i = \text{t}_v_i$ into Eq. (22) and, using Eq. (4), equation (22) is simplified to give the Eulerian form of the dynamic equation of motion as given below:

$$\begin{aligned} & \int_{\text{t}_V} \frac{\partial \delta u_i}{\partial \text{t}_x^j} (\text{t}_i \dot{\sigma}_{ij} - v_k \frac{\partial \text{t}_i \sigma_{ij}}{\partial \text{t}_x^k}) \text{t}_V dV + \int_{\text{t}_V} \delta u_i [(\text{t}_i \rho \dot{v}_i) - \text{t}_v_k \frac{\partial (\text{t}_i \rho \dot{v}_i)}{\partial \text{t}_x^k}] \text{t}_V dV \\ & = \int_{\text{t}_V} \delta u_i [(\text{t}_i f_i^B \text{t}_i \rho) - \text{t}_v_k \frac{\partial (\text{t}_i f_i^B \text{t}_i \rho)}{\partial \text{t}_x^k}] \text{t}_V dV + \int_{\text{t}_A} \delta u_i \text{t}_i f_i^s \text{t}_A dA \end{aligned} \quad (26)$$

This equation is the linearized form of the general equation of conservation of momentum in Eulerian view [23].

It is noted that in the ALE equation of motion (equation 22), terms exist that involve spatial gradients of stress. These gradients give rise to convective terms in the final equations involving product of stress gradients and convective velocity, and may lead to the numerical instability of the solution. Handling such terms in the solution of ALE equations requires special treatment. Various treatments have been used in the literature to overcome this difficulty. Liu et al. [25] introduced a stress-velocity product which converts the computation of the stress gradient into the computation of gradient of stress-velocity product. Later, Liu et al. [11] included an artificial viscosity term to deal with oscillations in the solution (streamline upwind method). Ghosh and Kicuchi [10] neglected these convective terms arguing that in solid mechanics problems not involving impact or shock, these terms are not significant. Hutienk [24] introduced a method for finding continuous stress field by extrapolation from integration points to nodal points. He used a least square method for averaging the stress values on the element boundaries. This method is popular in the ALE literature, though it involves large approximations. Bayoumi et al. [6] avoided the calculation of stress gradients by using the divergence theorem to transform the volume integrals into surface integrals. We follow the latter approach here in dealing with stress gradients. First, integration by part is used to get a form suitable for applying the divergence theorem;

$$\begin{aligned} & \int_{\text{t}_V} \frac{\partial \delta u_i}{\partial \text{t}_x^j} (u_k - u_k^g) \frac{\partial \text{t}_i \sigma_{ij}}{\partial \text{t}_x^k} \text{t}_V dV = \int_{\text{t}_V} \frac{\partial}{\partial \text{t}_x^j} \left[\frac{\partial \delta u_i}{\partial \text{t}_x^k} (u_k - u_k^g) \text{t}_i \sigma_{ij} \right] \text{t}_V dV - \\ & \int_{\text{t}_V} \frac{\partial^2 \delta u_i}{\partial \text{t}_x^k \partial \text{t}_x^j} (u_k - u_k^g) \text{t}_i \sigma_{ij} \text{t}_V dV - \int_{\text{t}_V} \frac{\partial \delta u_i}{\partial \text{t}_x^j} \frac{\partial (u_k - u_k^g)}{\partial \text{t}_x^k} \text{t}_i \sigma_{ij} \text{t}_V dV \end{aligned} \quad (27)$$

Next, the divergence theorem is used to convert the first integral in the right-hand side of Eq. (27) to surface integral and the boundary constraint Eq. (1) is applied. It is noted that the latter equation is in terms of velocity components and must be written in terms of displacements first. This can be achieved by multiplying both sides of the equation by Δt . This approximation is consistent with the incremental solution [1, 6]. Therefore,

$$\int_{\text{t}_V} \frac{\partial \delta u_i}{\partial \text{t}_x^j} (u_k - u_k^g) \frac{\partial \text{t}_i \sigma_{ij}}{\partial \text{t}_x^k} \text{t}_V dV = - \int_{\text{t}_V} \frac{\partial^2 \delta u_i}{\partial \text{t}_x^k \partial \text{t}_x^j} (u_k - u_k^g) \text{t}_i \sigma_{ij} \text{t}_V dV - \int_{\text{t}_V} \frac{\partial \delta u_i}{\partial \text{t}_x^j} \frac{\partial (u_k - u_k^g)}{\partial \text{t}_x^k} \text{t}_i \sigma_{ij} \text{t}_V dV \quad (28)$$

A similar treatment is used to simplify terms that involve gradients of density in the relevant terms of Eq. (22). Inserting this modified Eq. into (22), the final form of ALE equation is obtained

$$\begin{aligned}
 & \int_V \frac{\partial \delta u_i}{\partial x_j} ({}^t \sigma_{ij} \Delta t - {}^t \sigma_{ik} \frac{\partial u_j^g}{\partial x_k} + {}^t \sigma_{ij} \frac{\partial u_k}{\partial x_k}) {}^t dV + \int_V \frac{\partial^2 \delta u_i}{\partial x_k \partial x_j} ({}^t u_k - {}^t u_k^g) {}^t \sigma_{ij} {}^t dV \\
 & \int_V \delta u_i {}^{t+\Delta t} v_i' {}^t \rho {}^t dV + \int_V \delta u_i {}^t c_j \frac{\partial {}^{t+\Delta t} v_i}{\partial x_j} {}^t \rho {}^t dV = \\
 & \delta {}^{t+\Delta t} W^{ext} - \int_V {}^t \sigma_{ij} \frac{\partial \delta u_i}{\partial x_j} {}^t dV - \int_V {}^t \rho {}^t c_j \frac{\partial (\delta u_i {}^t v_i')}{\partial x_j} {}^t dV \Delta t - \int_V \delta u_i {}^t c_j' \frac{\partial {}^t v_i}{\partial x_j} {}^t \rho {}^t dV \Delta t + \\
 & \int_V \delta u_i {}^t c_j \frac{\partial {}^t v_i}{\partial x_k} \frac{\partial {}^t v_k^g}{\partial x_j} {}^t \rho {}^t dV \Delta t - \int_V {}^t \rho {}^t c_j \frac{\partial}{\partial x_j} (\delta u_i {}^t c_k \frac{\partial {}^t v_i}{\partial x_k}) {}^t dV \Delta t
 \end{aligned} \tag{29}$$

Where

$$\begin{aligned}
 \delta {}^{t+\Delta t} W^{ext} &= \int_V \delta u_i ({}^t f_i^B + f_i^B) {}^t \rho {}^t dV + \int_V {}^t \rho (u_k - u_k^g) \frac{\partial}{\partial x_k} [\delta u_i ({}^t f_i^B + f_i^B)] {}^t dV + \\
 & \int_A \delta u_i ({}^t f_i^S + f_i^S) {}^t dA + \int_A \delta u_i {}^t f_i^S \left[\frac{\partial u_k^g}{\partial x_k} - \frac{1}{2} {}^t n_m \left(\frac{\partial u_m^g}{\partial x_n} + \frac{\partial u_n^g}{\partial x_m} \right) {}^t n_n \right] {}^t dA
 \end{aligned} \tag{30}$$

It is noted that although Eqs. (29) and (30) do not involve gradients of stress, they involve the second derivatives of displacements, which requires that elements with C1-continuity are used for the finite element discretization.

c) Incremental form of energy equation

Equation (17) expresses the temperature gradient in the ALE frame system. By substituting this form into the equation of balance of energy given in Eq. (10), the ALE form of the equation of energy is obtained as:

$$\begin{aligned}
 & \int_{t+\Delta V} \delta T {}^{t+\Delta t} c_p {}^{t+\Delta t} T {}^{t+\Delta t} \rho {}^{t+\Delta t} dV + \int_{t+\Delta V} \delta T {}^{t+\Delta t} c_p {}^{t+\Delta t} c_j \frac{\partial {}^{t+\Delta t} T}{\partial x_j} {}^{t+\Delta t} \rho {}^{t+\Delta t} dV + \\
 & \int_{t+\Delta V} \frac{\partial \delta T}{\partial x_i} {}^{t+\Delta t} k_{ij} \frac{\partial {}^{t+\Delta t} T}{\partial x_j} {}^{t+\Delta t} dV = \int_{t+\Delta V} \delta T {}^{t+\Delta t} \rho {}^{t+\Delta t} r {}^{t+\Delta t} dV + \\
 & \int_{t+\Delta V} \delta T {}^{t+\Delta t} \dot{W}^{irr} {}^{t+\Delta t} dV - \int_{t+\Delta S} \delta T {}^{t+\Delta t} q_i {}^{t+\Delta t} n_i {}^{t+\Delta t} dS
 \end{aligned} \tag{31}$$

Furthermore, the spatial derivatives of temperature with respect to spatial coordinates at time $t + \Delta t$ may be expressed in terms of spatial coordinates at time t as follows (Eq. (16))

$$\frac{\partial {}^{t+\Delta t} T}{\partial x_j} = \frac{\partial {}^{t+\Delta t} T}{\partial x_j} - \frac{\partial {}^{t+\Delta t} T}{\partial x_k} \frac{\partial v_k^g}{\partial x_j} \Delta t \tag{32}$$

Substituting Eq. (32) into the second and the third terms of the left-hand side of Eq. (31) and neglecting higher order terms, we get

$$\begin{aligned}
 & \int_{t+\Delta V} \delta T {}^{t+\Delta t} c_p {}^{t+\Delta t} T {}^{t+\Delta t} \rho {}^{t+\Delta t} dV + \int_{t+\Delta V} \delta T {}^{t+\Delta t} c_p {}^{t+\Delta t} c_j \frac{\partial {}^{t+\Delta t} T}{\partial x_j} {}^{t+\Delta t} \rho {}^{t+\Delta t} dV + \\
 & \int_{t+\Delta V} \frac{\partial \delta T}{\partial x_i} {}^{t+\Delta t} k_{ij} \frac{\partial {}^{t+\Delta t} T}{\partial x_j} {}^{t+\Delta t} dV = \int_{t+\Delta V} \delta T {}^{t+\Delta t} \rho {}^{t+\Delta t} r {}^{t+\Delta t} dV + \int_{t+\Delta V} \delta T {}^{t+\Delta t} \dot{W}^{irr} {}^{t+\Delta t} dV - \\
 & \int_{t+\Delta S} \delta T {}^{t+\Delta t} q_i {}^{t+\Delta t} n_i {}^{t+\Delta t} dS + \left[\int_{t+\Delta V} \delta T {}^{t+\Delta t} c_p {}^{t+\Delta t} c_j \frac{\partial {}^{t+\Delta t} T}{\partial x_k} \frac{\partial v_k^g}{\partial x_j} {}^{t+\Delta t} \rho {}^{t+\Delta t} dV \right] \Delta t + \\
 & \left[\int_{t+\Delta V} \frac{\partial \delta T}{\partial x_i} {}^{t+\Delta t} k_{ij} \frac{\partial {}^{t+\Delta t} T}{\partial x_k} \frac{\partial v_k^g}{\partial x_j} {}^{t+\Delta t} dV + \int_{t+\Delta V} \frac{\partial \delta T}{\partial x_k} \frac{\partial v_k^g}{\partial x_i} {}^{t+\Delta t} k_{ij} \frac{\partial {}^{t+\Delta t} T}{\partial x_j} {}^{t+\Delta t} dV \right] \Delta t
 \end{aligned} \tag{33}$$

It is noted that the above equation represents a coupled ALE energy equation in the sense that simultaneous motion of material and grid are considered in the formulation through introduction of Eq. (17). However, due to the staggered solution algorithm used with respect to the deformation-thermal sequence of solution, the temperature variables are expressed at time $t + \Delta t$. More details on this solution algorithm are given in section 4.2.

d) Features of the new formulation

The thermo-mechanical ALE formulation presented above has a feature that distinguishes it from similar ALE formulations in the literature. Here, we point out some of these differences.

1- The formulation represents a fully coupled ALE analysis because it implements simultaneous motion of material and grid points. In this sense, it differs from the ALE formulations that use operator split approach. This is true for the thermal part of the formulation too, because convective terms describing the relation between material and grid motions appear in the formulation. To our knowledge, this type of treatment of the energy equation has not been presented before.

2- A similar treatment of ALE equation of motion has been previously presented by Wang et al. [5] for quasi-static analysis and by Bayoumi and Gadala [6, 1] for dynamic analysis. However, the present formulation differs from the latter work in that it has been considerably simplified in the following points:

a) In reference [6], linearization of equation of motion is carried out using the relationships: ${}^{t+\Delta t}v_i^g = {}^t v_i^g + \dot{v}_i^g$ and ${}^{t+\Delta t}v_i = {}^t v_i + \dot{v}_i$. Later, the incremental material and grid velocities are linearized again to yield displacements. In other words, linearization is performed twice to relate the convective velocity at time $t + \Delta t$ to displacement at time t . This operation has introduced an extra term to the final equation.

b) In the dynamic analysis, it is not usually necessary to linearize the velocity and acceleration at time $t + \Delta t$ because the time incrementation of the velocity, and acceleration at time $t + \Delta t$ is achieved using methods such as Newmark's. Unlike reference [6], here, velocities and accelerations at time $t + \Delta t$ are maintained in the equation during linearization. Then, after discretization of the equation, the Newmark method is used to obtain the time marching form of the equation. This general method reduces the computational time considerably, as the calculations to obtain the relationships between incremental displacements, velocities, and accelerations for the material and the grid in the Newmark approach are avoided.

4. IMPLEMENTATION OF THERMO-ELASTO-VISCOPLASTIC MATERIAL MODELS

For thermo-mechanical simulation of material behavior, a comprehensive material model that includes the effects of strain, strain rate and temperature is often used. In this section, a thermo-viscoplastic continuum modulus based on the consistency model is presented, and an algorithmic tangent modulus is developed which facilitates the updating of stresses at a faster rate of convergence.

a) Derivation of continuum modulus

In finite strain viscoplasticity, there are two common models to deal with the viscoplastic effects; the overstress model [26, 27, 28] and the consistency model [18, 29, 30, 31]. In this paper, we use the consistency model based on reference [13] and develop the required algorithmic modulus for ALE analysis. The development is based on Mises plasticity with isotropic hardening. The yield function is expressed as a function of stress, equivalent plastic strain, equivalent plastic strain rate and temperature;

$$f = \bar{\sigma} - \sigma_Y (\bar{\varepsilon}^p, \dot{\bar{\varepsilon}}^p, T) \quad (34)$$

where $\bar{\sigma}$ is the equivalent stress expressed in terms of deviatoric stress \mathbf{S} and $\dot{\bar{\epsilon}}^p$ is the equivalent plastic strain rate which can be defined as

$$\bar{\sigma} = \sqrt{\frac{3}{2} \mathbf{S} : \mathbf{S}} \quad (35)$$

$$\dot{\bar{\epsilon}}^p = \sqrt{\frac{2}{3} \mathbf{D}^p : \mathbf{D}^p} \quad (36)$$

For hypoelasto-plastic materials, an additive decomposition of the rate of deformation tensor \mathbf{D} is often used [32]:

$$\mathbf{D} = \mathbf{D}^e + \mathbf{D}^T + \mathbf{D}^p \quad (37)$$

where \mathbf{D}^e and \mathbf{D}^p are the elastic and plastic part of the deformation tensor, and \mathbf{D}^T is the thermal strain rate for isotropic materials expressed as

$$\mathbf{D}^T = \alpha \dot{T} \mathbf{I} \quad (38)$$

where \mathbf{I} is unit second order tensor and α is coefficient of thermal expansion. In large deformation analysis, an objective stress rate should be used to provide the objectivity of constitutive equation. The elastic stress-strain relation may be written as

$$\overset{\nabla}{\boldsymbol{\sigma}} = \mathbf{C}^{ep} : \mathbf{D} + \boldsymbol{\Sigma} \dot{T} \quad (39)$$

where \mathbf{C}^{ep} and $\boldsymbol{\Sigma}$ are:

$$\mathbf{C}^{ep} = \mathbf{C}^e - \mathbf{C}^p = \mathbf{C}^e - \frac{4G^2}{H} \mathbf{N} \otimes \mathbf{N} \quad (40)$$

$$\boldsymbol{\Sigma} = \frac{2G}{H} \frac{\partial \sigma_Y}{\partial T} \mathbf{N} - \mathbf{C}^{ep} : \mathbf{I} \alpha \quad (41)$$

where G is the shear modulus and the hardening parameter H is expressed as

$$H = 3G + \frac{\partial \sigma_Y}{\partial \bar{\epsilon}^p} + \left(\frac{1}{\Delta t} \right) \frac{\partial \sigma_Y}{\partial \dot{\bar{\epsilon}}^p} \quad (42)$$

b) Stress updating algorithm

A major challenge in large deformation analysis is the time integration of the constitutive equation in a way that the stress update algorithm maintains incremental objectivity. For elastic-plastic materials, the plastic consistency condition should always be satisfied, i.e., the stress state at the end of the integration time step should conform to the yield surface. Here, the classic return mapping algorithm is extended for finite viscoplastic deformation. The method consists of an elastic predictor step in which a trial stress at time $t+\Delta t$ is computed by assuming pure elastic deformation, followed by a plastic corrector step in which the stress state is projected on the updated yield surface to satisfy the plastic consistency condition. This method is widely used in Lagrangian solutions in which the integration points are attached to the material points. However, in an ALE solution, the integration points are convected and may represent different material points during the deformation. Because of this convective effect, the stress update may not be performed as in a Lagrangian formulation. The strategies proposed for handling the convective

terms are different in split and unsplit ALE approaches as detailed in reference [12]. The stress updating procedure used here is an unsplit version of return mapping algorithm based on incremental decomposition of stress in ALE form:

$${}^{t+\Delta t}\sigma_{ij} = {}^t\sigma_{ij} + {}^t\dot{\sigma}_{ij}\Delta t - (u_k - u_k^g) \frac{\partial {}^t\sigma_{ij}}{\partial {}^t x_k} \quad (43)$$

Using an objective stress rate, e.g. Jaumann rate, Eq. (43) may be expressed as [12]

$${}^{t+\Delta t}\sigma_{ij} = {}^t\sigma_{ij} + \Delta\sigma_{ij}^{rota} + \Delta\sigma_{ij}^{conv} + {}^tC_{ijkl} {}^tD_{kl} \Delta t \quad (44)$$

where $\Delta\sigma_{ij}^{rota}$ represents a rotational objective term given by

$$\Delta\sigma_{ij}^{rota} = \frac{\partial u_i}{\partial {}^t x_n} {}^t\sigma_{nj} + \frac{\partial u_j}{\partial {}^t x_m} {}^t\sigma_{im} - \frac{\partial u_k}{\partial {}^t x_k} {}^t\sigma_{ij} \quad (45)$$

and $\Delta\sigma_{ij}^{conv}$ is the ALE convective term given by

$$\Delta\sigma_{ij}^{conv} = -(u_k - u_k^g) \frac{\partial {}^t\sigma_{ij}}{\partial {}^t x_k} \quad (46)$$

In other words, the equation (44) may be regrouped into predictor and corrector terms:

$${}^{t+\Delta t}\sigma_{ij} = \Delta\sigma_{ij}^{pred} + \Delta\sigma_{ij}^{corr} + \Delta\sigma_{ij}^{conv} \quad (47)$$

where $\Delta\sigma_{ij}^{pred}$ is the elastic predictor trial stress given by

$$\Delta\sigma_{ij}^{pred} = {}^t\sigma_{ij} + \Delta\sigma_{ij}^{rota} + {}^tC_{ijkl} {}^tD_{kl} \Delta t \quad (48)$$

and $\Delta\sigma_{ij}^{corr}$ is the plastic corrector stress increment given by

$$\Delta\sigma_{ij}^{corr} = -{}^tC_{ijkl} {}^tD_{kl}^p \Delta t \quad (49)$$

The convective term may be included in either the predictor step, the corrector step or in both. In this work, the convective term is used in both predictor and corrector steps of the return mapping algorithm, because in our experiments, it yielded more stable results. Finally, it is noted that although the above updating algorithm is in principle a return mapping algorithm, the equation derived for the predictor step is different from that used in Lagrangian analysis. Thus, a new consistent elasto-viscoplastic tangent modulus should be developed.

c) Consistent elasto-viscoplastic tangent modulus

In an implicit solution method, an appropriate tangent modulus is needed. For this purpose, an algorithmic tangent modulus based on systematic linearization of the constitutive equations is developed here. This modulus is preferred over the continuum elasto-plastic tangent modulus because the latter modulus can cause spurious loading and unloading in transition to the plastic zone. Furthermore, it is shown that an asymptotic rate of quadratic convergence is achieved when an algorithmic modulus is used [33]. The algorithmic tangent modulus for backward Euler update is defined as

$$d \overset{\nabla}{\sigma} = \mathbf{C}^{alg} : d\mathbf{D} \quad (50)$$

The stress increment can be expressed in terms of elastic part of rate of deformation

$$d \overset{\nabla}{\boldsymbol{\sigma}} = \mathbf{C}^e : (d\mathbf{D} - d\mathbf{D}^p - d\mathbf{D}^T) \quad (51)$$

$$d\mathbf{D}^p = (d\dot{\lambda})\mathbf{N} + \dot{\lambda}(d\mathbf{N}) \quad (52)$$

$$d\dot{\lambda} = \frac{2G}{H}(d\mathbf{N} : \mathbf{D} + \mathbf{N} : d\mathbf{D}) \quad (53)$$

The derivative of \mathbf{N} may be defined as

$$d\mathbf{N} = \mathbf{Z} : d\boldsymbol{\sigma} \quad (54)$$

where

$$\mathbf{Z} = \frac{\sqrt{3/2}}{\sqrt{\mathbf{S} : \mathbf{S}}}(\mathbf{I}^{dev} - \hat{\mathbf{N}} \otimes \hat{\mathbf{N}}) \quad (55)$$

and

$$\hat{\mathbf{N}} = \sqrt{\frac{2}{3}}\mathbf{N} \quad (56)$$

Cauchy stress tensor in the current configuration is written as

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^{trial} - 2G\dot{\lambda}\mathbf{N} = \boldsymbol{\sigma}^{trial} - \mathbf{C}^e : \mathbf{D}^p \quad (57)$$

For a constant elastic parameter, the stress increment is given by

$$d\boldsymbol{\sigma} = d\boldsymbol{\sigma}^{trial} - \mathbf{C}^e : d\mathbf{D}^p \quad (58)$$

In order to obtain $\boldsymbol{\sigma}^{trial}$, the objective predictor elastic stress (Eq. (48)) is used to develop a new consistent, elasto-viscoplastic tangent modulus which has a simple form and can be readily implemented in an FE program. Differentiating $\boldsymbol{\sigma}^{trial}$ as given below

$$d\boldsymbol{\sigma}^{trial} = 2Gd\mathbf{D} + d\mathbf{L}\boldsymbol{\sigma} + \boldsymbol{\sigma}d\mathbf{L} - \boldsymbol{\sigma}(\mathbf{I} : d\mathbf{D}) \quad (59)$$

and substituting (59), (58) and (54) into (53),

$$d\dot{\lambda} = \frac{2G}{H}\{[2G\mathbf{D} : \mathbf{Z} + \mathbf{N} + (\mathbf{D} : \mathbf{Z})\boldsymbol{\sigma} + \boldsymbol{\sigma}(\mathbf{D} : \mathbf{Z}) - ((\mathbf{D} : \mathbf{Z}) : \boldsymbol{\sigma})\mathbf{I}] : d\mathbf{D} - (\mathbf{D} : \mathbf{Z}) : d\mathbf{D}^p\} \quad (60)$$

Substituting Eq. (60) in (52):

$$d\mathbf{D}^p = 2G(\mathbf{T}^{-1} : \mathbf{P}) : d\mathbf{D} \quad (61)$$

where tensors \mathbf{T} and \mathbf{P} are defined as

$$\mathbf{T} = \mathbf{I} + \frac{2G}{H}[(\mathbf{C}^e : \mathbf{Z}) : \mathbf{D}] \otimes \mathbf{N} + \dot{\lambda}\mathbf{Z} : \mathbf{C}^e \quad (62)$$

$$\mathbf{P} = \frac{2G}{H}[2G\mathbf{D} : \mathbf{Z} + \mathbf{N} + (\mathbf{D} : \mathbf{Z})\boldsymbol{\sigma} + \boldsymbol{\sigma}(\mathbf{D} : \mathbf{Z}) - ((\mathbf{D} : \mathbf{Z}) : \boldsymbol{\sigma})\mathbf{I}] \otimes \mathbf{N} + \dot{\lambda}[2G\mathbf{Z} + \mathbf{Z}\boldsymbol{\sigma} + \boldsymbol{\sigma}\mathbf{Z} - (\mathbf{Z}\boldsymbol{\sigma})\mathbf{I}] \quad (63)$$

By simplifying Eq. (62) through a long algebraic manipulation, one gets:

$$\mathbf{T}^{-1} = [\mathbf{C}^e - 2Gb\hat{\mathbf{I}}]\mathbf{C}^{e-1} \quad (64)$$

Parameter b and tensor $\hat{\mathbf{I}}$ are expressed as:

$$b = \frac{2Ga}{2Ga + 1} \quad (65)$$

$$a = \dot{\lambda} \frac{\sqrt{3/2}}{\sqrt{\mathbf{S}^{trail} : \mathbf{S}^{trail}}} \quad (66)$$

$$\hat{\mathbf{I}} = \mathbf{I}^{dev} - 2\hat{\mathbf{N}} \otimes \hat{\mathbf{N}} \quad (67)$$

Combining Eqs. (64), (63), (61) and (51), the final form of the tangent modulus is obtained as

$$\mathbf{C}^{alg} = \left[\mathbf{C}^e - 2G \left(\mathbf{T}^{-1} : \mathbf{P} \right) \right] \quad (68)$$

5. CONCLUSION

In this paper, a fully coupled ALE formulation is presented for simulation of large deformation thermo-mechanical problems. The governing equation of deformation and energy balance in the ALE frame of reference are derived. The features of this formulation compared to similar formulations in the literature are described. A continuum modulus for implementation of rate and temperature dependent constitutive equations is developed. The versatility of the formulation makes it suitable for simulation of large deformation of materials under dynamic loads, high strain rate and high temperatures. In the second part of this paper series, implementation of this formulation in finite element analysis is presented and example problems are solved to verify the capabilities of the given formulation.

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