A Thermodynamic Framework for Rate-Independent Dissipative Materials with Internal Functions

by

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ABSTRACT

This paper builds on previous work (Houlsby and Puzrin, 1998) in which a framework was set out for the derivation of rate-independent plasticity theory from thermodynamic considerations. A key feature of the formalism is that the entire constitutive response is determined by knowledge of two scalar functions. The loading history is effectively captured through the use of internal variables. In this paper we extend the concept of internal variables to that of internal functions, which represent infinite numbers of internal variables. In this case the thermodynamic functions are replaced by functionals. We set out the formalism necessary to derive constitutive behaviour within this approach. The principal advantages of this development is that it can provide realistic modelling of kinematic hardening effects and smooth transitions between elastic and elastic-plastic behaviour.

INTRODUCTION

Houlsby and Puzrin (1998) set out a general framework for the derivation of the constitutive behaviour of rate independent elastic-plastic materials within the setting of thermodynamics. A key element of the approach that they developed was that the constitutive behaviour is entirely specified by the knowledge of two functions: an energy function and either the dissipation function or the yield function. They set out how the incremental constitutive behaviour could be derived from these functions. They also explored the relationships between alternative forms of the energy functions, and between the dissipation and yield functions. Legendre transformaions played a central role in achieving these relations.

This paper builds entirely on the results of Houlsby and Puzrin (1998) (hereinafter abbreviated to H&P), and much cross reference to that paper is necessary to avoid this paper becoming excessively long. In particular equation numbers in H&P will be referred to in the form “Eq. (H&P) 1.2.3”. The results in H&P in turn build principally on material presented by Collins and Houlsby (1997), in which the methods proposed by Ziegler (1977) are applied to rate-independent materials. H&P discuss the role of Ziegler’s “orthogonality” principle. Further useful discussion of this topic can be found in Rajagopal and Srinivasa (1998a,b).

The theoretical approaches to the mechanics of inelastic materials can be divided into two main classes, which are often termed generalised thermodynamics and rational mechanics. The generalised thermodynamics approach (which is used here) makes much use of internal variables to describe the history of loading, and the current response is expressed in terms of functions of the stress and/or strain state and the internal variables. The rational mechanics approach (see for example Truesdell (1977)) instead expresses the response in terms of functionals of the history of the material (usually through the history of strain and

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temperature). Both approaches have advantages and drawbacks. Rational mechanics achieves
great generality, but at the expense that it has so far proved difficult to express simple material
models for inelastic materials within this framework. Generalised thermodynamics has been a
very successful framework for simple models, but has the disadvantage that the use of internal
variables sometimes over-simplifies the response. In particular it is difficult to express smooth
transitions of behaviour using internal variables. In this paper we address this shortcoming of
generalised thermodynamics by extending the concept of internal variable to that of internal
function. The response is then expressed in terms of functionals, and so offers some of the
advantages achieved by rational mechanics. Indeed it is hoped that this approach may in due
course provide some link between the two frameworks of generalised thermodynamics and
rational mechanics.

In this paper we need to make use of certain mathematical techniques which may be
unfamiliar to readers. We include therefore Appendices on these techniques. In particular we
have to make use of the generalisation of the concept of the differential of a to that of the
Frechet differential. We also make extensive use of Legendre Transformations. Collins and
Houlsby (1997) provide an Appendix on the use of Legendre Transformations of the type used
by H&P. In the appendices here we consider the case of Legendre Transformations of
functionals (rather than functions).

As was the case in H&P, we develop results here for the case of small strain analysis, and
express these using Cartesian tensors with subscript notation. Although the results could in
principle be extended to large strain, the complexities that this introduces should not be
underestimated.

PLASTICITY MODELS WITH MULTIPLE INTERNAL VARIABLES

For simplicity, H&P considered materials which could be characterised by a single kinematic
internal variable $\alpha_{ij}$, which was in the form of a second order tensor. The kinematic internal
variable can often be conveniently identified with the plastic strain. The significance of the
single internal variable is that a single yield surface is derived, on which there is an abrupt
change from elastic to elastic-plastic behaviour. The generalisation of the results to some other
cases is straightforward, for instance the case of a scalar internal variable can be obtained
simply by dropping the subscripts from the variables $\alpha_{ij}, \chi_{ij}$ and $\bar{\chi}_{ij}$ in H&P.

The generalisation to some more complex cases is marginally more complex. For instance the
case of $N$ second order tensor internal variables would mean that the function for the Gibbs
free energy $g(\sigma_{ij}, \alpha_{ij}, \theta)$ in H&P is simply generalised to $g(\sigma_{ij}, \alpha_{ij}^{(1)}, \ldots, \alpha_{ij}^{(N)}, \theta)$. The
corresponding differential $\chi_{ij} = -\frac{\partial g}{\partial \alpha_{ij}}$ is replaced by $\chi_{ij}^{(n)} = -\frac{\partial g}{\partial \alpha_{ij}^{(n)}}$, where $n = 1 \ldots N$. The
corresponding forms and results for other energy functions and differentials follow a similar
pattern. In principle, when Legendre transformations are made between different functions,
the number of possible transformations becomes enormous (for instance there are $2^{(2+N)}$
possible forms of the energy function). In practice, however, it is likely that only a small
fraction of the possible forms would be of practical application, and so no systematic
presentation of the forms with multiple internal variables is given here.
If any of the $N$ internal variables are scalars rather than tensors, then all that is necessary is again to drop the subscripts from the appropriate variables.

The main reason for the introduction of multiple internal variables is to allow the definition of models with multiple yield surfaces. These can be used for a variety of purposes, e.g.:

- modelling separately compression and shear effects, as may be appropriate for some granular materials (i.e., “cone and cap” models),
- modelling anisotropy through use of multiple kinematically hardening yield surfaces,
- approximation of a smooth transition from elastic to plastic behaviour.

The last of these purposes is perhaps the most important. The use of internal variables (within the thermodynamic framework) is an extremely powerful method for describing the past history of an elastic-plastic material, but suffers from the disadvantage that it inevitably leads to abrupt changes between elastic and elastic-plastic behaviour. Although use of multiple internal variables allows these changes to be divided into a number of smaller steps, a completely smooth transition can only be achieved by introducing an infinite number of internal variables. Such an idea leads to the concept of an internal function rather than internal variables. The generalisation of the results given by H&P to the case of internal functions is rather more complex than the generalisations discussed above, and is the subject of this paper.

In general the internal function will be expressed in terms of a variable $\eta$ which we will term the internal co-ordinate, so we write the internal function as $\hat{\alpha}_{ij}(\eta)$. In many cases $\eta$ will not have any obvious physical interpretation, but in some cases it may.

We use the “hat” notation to distinguish any variable which is a function of the internal co-ordinate from a previously used variable with the same name.

H&P developed a general formulation in which a number of alternative forms of energy functions were used. We shall here pursue only one of these alternatives. Other forms can be obtained by analogous developments of the work of H&P. We take the example of the Gibbs free energy. The free energy function will now become a free energy functional

$$g[\sigma_{ij}, \hat{\alpha}_{ij}(\eta), \theta] = \int_{Y} \hat{g}(\sigma_{ij}, \hat{\alpha}_{ij}(\eta), \theta, \eta) \Gamma(\eta) \, d\eta$$

(1)

where $Y$ is the domain of $\eta$. Other more general forms of functional are of course possible, but the form in Eq. 1 proves to be of practical use and importance. It is convenient to introduce for generality the (non-negative) weighting function $\Gamma(\eta)$ within the integral in Eq. 1.

In some cases it may be more convenient to consider the free energy as the sum of a function and a functional:
\[ g[\sigma_{ij}, \dot{\alpha}_{ij}, \theta] = g_1(\sigma_{ij}, \theta) + \int_Y \hat{g}_2(\sigma_{ij}, \dot{\alpha}_{ij}(\eta), \theta, \eta) \Gamma(\eta) d\eta \] (2)

For simplicity, however, we shall first describe just the functional form (Eq. 1) here. In any case, \( g_1 \) in Eq. 2 can be included with \( \hat{g}_2 \) within the integral simply by dividing by the constant \( \int_Y \Gamma(\eta) d\eta \).

**Generalised Stress**

H&P make use of a generalised stress, which is work-conjugate to the internal kinematic variable and is defined by \( \tilde{\chi}_{ij} = -\frac{\partial g}{\partial \alpha_{ij}} \). Corresponding therefore to the kinematic internal function is a *generalised stress function* \( \hat{\chi}_{ij}(\eta) \). For the single internal variable it is easy to show (using definitions in H&P) that:

\[ \dot{g} = -\varepsilon_{ij} \sigma_{ij} - \tilde{\chi}_{ij} \dot{\alpha}_{ij} - s\dot{\theta} \] (3)

For the case with multiple internal variables this simply becomes:

\[ \dot{g} = -\varepsilon_{ij} \sigma_{ij} - \sum_{n=1}^{N} \tilde{\chi}_{ij}^{(n)} \dot{\alpha}_{ij}^{(n)} - s\dot{\theta} \] (4)

Generalising for the case of the functional, this in turn becomes:

\[ \dot{g} = -\varepsilon_{ij} \sigma_{ij} - \int_Y \tilde{\chi}_{ij}(\eta) \dot{\alpha}_{ij}(\eta) \Gamma(\eta) d\eta - s\dot{\theta} \] (5)

By making use of the generalisation of the concept of the differential to that of the Frechet differential (see Appendix 1, eq. A1b2), Eq. 5 leads to the result:

\[ \hat{\chi}_{ij} = -\frac{\partial \hat{g}}{\partial \alpha_{ij}} \] (6)

We shall in fact adopt Eq. 6 as the definition of the generalised stress function \( \hat{\chi}_{ij} \).

**Dissipation functional**

H&P define a dissipation function. In a similar way we can write a *dissipation functional* in the form:

\[ d^g[\sigma_{ij}, \dot{\alpha}_{ij}, \theta, \dot{\alpha}_{ij}] = \int_Y d^g(\sigma_{ij}, \dot{\alpha}_{ij}(\eta), \theta, \dot{\alpha}_{ij}(\eta), \eta) \Gamma(\eta) d\eta \geq 0 \] (7)

Which can be compared with Eq. (H&P) 4.1.7.

Following the definition \( \chi_{ij} = \frac{\partial d^g}{\partial \alpha_{ij}} \), we shall define:
\[ \dot{\chi}_{ij} = \frac{\partial \dot{\alpha}^g}{\partial \dot{\alpha}_{ij}} \] (8)

Since \( \dot{\alpha}^g \) will be first order in \( \dot{\alpha}_{ij} \) for rate-independent materials, it follows that:

\[ \dot{\alpha}^g (\sigma_{ij}, \dot{\alpha}_{ij}(\eta), \theta, \dot{\alpha}_{ij}(\eta)) = \dot{\chi}_{ij}(\eta) \dot{\alpha}_{ij}(\eta) \] (9)

The considerations of thermodynamics leads to:

\[ d^g \left[ \sigma_{ij}, \dot{\alpha}_{ij}, \theta, \dot{\alpha}_{ij} \right] = \int_{\gamma} \ddot{\chi}_{ij}(\eta) \dot{\alpha}_{ij}(\eta) \Gamma(\eta) \kappa d\eta \] (10)

Equations 9 and 10 can be compared with Eq. (H&P) 4.1.6. It therefore follows that:

\[ \int_{\gamma} (\ddot{\chi}_{ij}(\eta) - \dot{\chi}_{ij}(\eta)) \dot{\alpha}_{ij}(\eta) \Gamma(\eta) \kappa d\eta = 0 \] (11)

Which compares with Eq. (H&P) 4.1.9. The generalised form of the orthogonality condition (or the constitutive hypothesis) therefore becomes simply \( \ddot{\chi}_{ij}(\eta) = \dot{\chi}_{ij}(\eta) \).

**Legendre transformations of the energy functional**

In the original approach a variety of Legendre transformations between energy functions were used, e.g. \( f(\epsilon_{ij}, \alpha_{ij}, \theta) = g(\sigma_{ij}, \alpha_{ij}, \theta) + \sigma_{ij} \epsilon_{ij} \). Transformations which involve variables (as opposed to functions of internal co-ordinate) are very similar to the original form, e.g. \( f(\epsilon_{ij}, \dot{\alpha}_{ij}, \theta) = g(\sigma_{ij}, \dot{\alpha}_{ij}, \theta) + \sigma_{ij} \epsilon_{ij} \). Those involving the internal function and the generalised stress function are slightly more complex. Thus instead of the original \( g(\sigma_{ij}, \alpha_{ij}, \theta) = g(\sigma_{ij}, \chi_{ij}, \theta) + \chi_{ij} \alpha_{ij} \) we have:

\[ \hat{g}(\sigma_{ij}, \dot{\alpha}_{ij}(\eta), \theta, \eta) = \hat{g}(\sigma_{ij}, \hat{\chi}_{ij}(\eta), \theta, \eta) + \hat{\chi}_{ij}(\eta) \alpha_{ij}(\eta) \] (12)

together with:

\[ \dot{\alpha}_{ij} = -\frac{\partial \hat{g}}{\partial \hat{\chi}_{ij}} \] (13)

(See Appendix 2 for details of the Legendre transformation methods for functionals).

We can also define:

\[ \hat{g}[\sigma_{ij}, \hat{\chi}_{ij}, \theta] = \int_{\gamma} \hat{g}(\sigma_{ij}, \hat{\chi}_{ij}(\eta), \theta, \eta) \Gamma(\eta) \kappa d\eta = g[\sigma_{ij}, \dot{\alpha}_{ij}, \theta] + \int_{\gamma} \hat{\chi}_{ij}(\eta) \alpha_{ij}(\eta) \Gamma(\eta) \kappa d\eta \] (14)

**Legendre transformation of the dissipation functional**

The only relevant transformation is the singular transformation from the dissipation functional to the yield functional. The original transformation was, for instance, of the form
\[ \lambda_y g^\eta \left( \sigma_{ij}, \alpha_{ij}, \theta, \chi_{ij} \right) = \chi_{ij} \lambda_y = \delta^g \left( \sigma^\eta, \alpha^\eta, \theta, \alpha^\eta \right) = 0 \], together with the result \( \lambda_{ij} = \frac{\lambda}{\partial \chi_{ij}}. \)

This now becomes (see Appendix 2(c)):

\[ \hat{\lambda}(\eta) \hat{y}^g \left( \sigma_{ij}, \hat{\alpha}_{ij}(\eta), \theta, \hat{\chi}_{ij}(\eta), \eta \right) = \hat{\chi}_{ij}(\eta) \hat{\alpha}_{ij}(\eta) - \frac{\partial}{\partial \eta} \left( \sigma_{ij}, \hat{\alpha}_{ij}(\eta), \theta, \hat{\alpha}_{ij}(\eta), \eta \right) = 0 \]  \hspace{1cm} (15)

together with the result that:

\[ \hat{\alpha}_{ij} = \hat{\lambda}(\eta) \frac{\partial \hat{y}}{\partial \hat{\chi}_{ij}} \]  \hspace{1cm} (16)

In principle is then possible to define a yield functional through adopting

\[ \lambda_y g^\eta \left[ \sigma_{ij}, \hat{\alpha}_{ij}, \theta, \hat{\chi}_{ij} \right] = \int_Y \hat{\lambda}(\eta) \hat{y}^g \left( \sigma_{ij}, \hat{\alpha}_{ij}(\eta), \theta, \hat{\chi}_{ij}(\eta) \right) \eta(\eta) d\eta = 0, \]  but it is unclear that this would serve any useful purpose.

**INCREMENTAL RESPONSE**

H&P showed how, given knowledge of the energy function and the yield function, it is possible to derive the entire incremental response for an elastic-plastic material within the formalism they adopted. This is of particular importance since non-linear material models are frequently implemented in finite element codes for which the incremental response is required.

The derivation of the incremental response begins with differentiation of the energy function, giving the results summarised in the sixth row of Table 1. Further differentiation gives the rates of the variables. This is set out for the single internal variable in general form as Eq. (H&P) 6.1.2, which for the particular case of the Gibbs free energy takes the form:

\[ \begin{bmatrix} -\dot{\varepsilon}_{ij} \\ -\dot{\chi}_{ij} \\ -\dot{s} \end{bmatrix} = \begin{bmatrix} \frac{\partial^2 g}{\partial \sigma_{ij} \partial \sigma_{kl}} & \frac{\partial^2 g}{\partial \sigma_{ij} \partial \alpha_{kl}} & \frac{\partial^2 g}{\partial \sigma_{ij} \partial \theta} \\ \frac{\partial^2 g}{\partial \alpha_{ij} \partial \sigma_{kl}} & \frac{\partial^2 g}{\partial \alpha_{ij} \partial \alpha_{kl}} & \frac{\partial^2 g}{\partial \alpha_{ij} \partial \theta} \\ \frac{\partial^2 g}{\partial \theta \partial \sigma_{kl}} & \frac{\partial^2 g}{\partial \theta \partial \alpha_{kl}} & \frac{\partial^2 g}{\partial \theta^2} \end{bmatrix} \begin{bmatrix} \dot{\sigma}_{kl} \\ \dot{\alpha}_{kl} \\ \dot{\theta} \end{bmatrix} \]  \hspace{1cm} (17)

This becomes in the new formulation:

\[ -\dot{\varepsilon}_{ij} = \int_Y \left( \frac{\partial^2 \hat{g}}{\partial \sigma_{ij} \partial \sigma_{kl}} \dot{\sigma}_{kl} + \frac{\partial^2 \hat{g}}{\partial \sigma_{ij} \partial \alpha_{kl}} \dot{\alpha}_{kl}(\eta) + \frac{\partial^2 \hat{g}}{\partial \sigma_{ij} \partial \theta} \dot{\theta} \right) \eta(\eta) d\eta \]  \hspace{1cm} (18)

\[ -\dot{\chi}_{ij}(\eta) = \frac{\partial^2 \hat{g}}{\partial \alpha_{ij} \partial \sigma_{kl}} \dot{\sigma}_{kl} + \frac{\partial^2 \hat{g}}{\partial \alpha_{ij} \partial \alpha_{kl}} \dot{\alpha}_{kl}(\eta) + \frac{\partial^2 \hat{g}}{\partial \alpha_{ij} \partial \theta} \dot{\theta} \]  \hspace{1cm} (19)
\[ -\dot{s} = \int \left( \frac{\partial^2 \dot{g}}{\partial \sigma_{ij} \partial \sigma_{kl}} \sigma_{ij} + \frac{\partial^2 \dot{g}}{\partial \theta \partial \alpha_{kl}} \dot{\alpha}_{kl}(\eta) + \frac{\partial^2 \dot{g}}{\partial \theta^2} \dot{\theta} \right) \Gamma(\eta) \eta \]  

(20)

Equations 18 to 20 are used together with the flow rule, Eq. 16 to derive:

\[ -\dot{\varepsilon}_{ij} = \int \left( \frac{\partial^2 \dot{g}}{\partial \sigma_{ij} \partial \sigma_{kl}} \sigma_{kl} + \frac{\partial^2 \dot{g}}{\partial \sigma_{ij} \partial \alpha_{kl}} \dot{\alpha}_{kl}(\eta) \frac{\partial \dot{\varepsilon}_{ij}}{\partial \lambda_{kl}} + \frac{\partial^2 \dot{g}}{\partial \sigma_{ij} \partial \theta} \dot{\theta} \right) \Gamma(\eta) \eta \]  

(21)

\[ -\dot{\lambda}_{ij}(\eta) = \frac{\partial^2 \dot{g}}{\partial \alpha_{ij} \partial \sigma_{kl}} \sigma_{kl} + \frac{\partial^2 \dot{g}}{\partial \alpha_{ij} \partial \alpha_{kl}} \dot{\alpha}_{kl}(\eta) \frac{\partial \dot{\lambda}_{ij}}{\partial \lambda_{kl}} + \frac{\partial^2 \dot{g}}{\partial \alpha_{ij} \partial \theta} \dot{\theta} \]  

(22)

\[ -\dot{s} = \int \left( \frac{\partial^2 \dot{g}}{\partial \theta \partial \sigma_{kl}} \sigma_{kl} + \frac{\partial^2 \dot{g}}{\partial \theta \partial \alpha_{kl}} \dot{\alpha}_{kl}(\eta) \frac{\partial \dot{\varepsilon}_{ij}}{\partial \lambda_{kl}} + \frac{\partial^2 \dot{g}}{\partial \theta^2} \dot{\theta} \right) \Gamma(\eta) \eta \]  

(23)

The infinitesimal multiplier function \( \dot{\lambda} \) is obtained by substitution of the above equations into the consistency condition, which is obtained by differentiation of the yield function. Eq. (H&P) 6.1.4 results in the condition:

\[ \dot{\varepsilon}^g = \frac{\partial \dot{g}}{\partial \sigma_{ij}} \sigma_{ij} + \frac{\partial \dot{g}}{\partial \alpha_{ij}} \dot{\alpha}_{ij} + \frac{\partial \dot{g}}{\partial \theta} \dot{\theta} + \frac{\partial \dot{g}}{\partial \lambda_{ij}} \dot{\lambda}_{ij} = 0 \]  

(24)

and for the functional approach this now becomes:

\[ \dot{\varepsilon}^g(\eta) = \frac{\partial \dot{g}}{\partial \sigma_{ij}} \sigma_{ij} + \frac{\partial \dot{g}}{\partial \alpha_{ij}} \dot{\alpha}_{ij}(\eta) + \frac{\partial \dot{g}}{\partial \theta} \dot{\theta} + \frac{\partial \dot{g}}{\partial \lambda_{ij}} \dot{\lambda}_{ij}(\eta) = 0 \]  

(25)

which leads immediately (on substitution of Eqs. 16 and 22) to:

\[ \frac{\partial \dot{g}}{\partial \sigma_{ij}} \sigma_{ij} + \frac{\partial \dot{g}}{\partial \alpha_{ij}} \dot{\alpha}_{ij}(\eta) \frac{\partial \dot{g}}{\partial \lambda_{ij}} + \frac{\partial \dot{g}}{\partial \theta} \dot{\theta} - \]  

\[ \frac{\partial \dot{g}}{\partial \lambda_{ij}} \left( \frac{\partial^2 \dot{g}}{\partial \alpha_{ij} \partial \sigma_{kl}} \sigma_{kl} + \frac{\partial^2 \dot{g}}{\partial \alpha_{ij} \partial \alpha_{kl}} \dot{\alpha}_{kl}(\eta) \frac{\partial \dot{g}}{\partial \lambda_{kl}} + \frac{\partial^2 \dot{g}}{\partial \alpha_{ij} \partial \theta} \dot{\theta} \right) = 0 \]  

(26)

From which we obtain:

\[ \dot{\lambda}(\eta) = \frac{\dot{\lambda}^\sigma(\eta)}{\dot{B}^g(\eta)} \sigma_{ij} - \frac{\dot{\lambda}^{\theta}(\eta)}{\dot{B}^g(\eta)} \dot{\theta} \]  

(27)

where

\[ \dot{\lambda}^\sigma(\eta) = \frac{\partial \dot{g}}{\partial \sigma_{ij}} - \frac{\partial \dot{g}}{\partial \lambda_{ij}} \frac{\partial^2 \dot{g}}{\partial \lambda_{kl} \partial \sigma_{ij}} \]  

(28)

\[ \dot{\lambda}^{\theta}(\eta) = \frac{\partial \dot{g}}{\partial \lambda_{ij}} - \frac{\partial \dot{g}}{\partial \lambda_{kl}} \frac{\partial^2 \dot{g}}{\partial \lambda_{kl} \partial \theta} \]  

(29)
\[ \hat{\mathbf{g}}(\eta) = \left( \frac{\partial g}{\partial \hat{\mathbf{g}}} - \frac{\partial \hat{\mathbf{g}}}{\partial \hat{\mathbf{g}}_{kl}} \frac{\partial^2 \hat{g}}{\partial \hat{\mathbf{g}}_{ij} \partial \hat{\mathbf{g}}_{kl} \partial \hat{\mathbf{g}}_{ij}} \right) \hat{\mathbf{g}}^{ij} \]  \hspace{1cm} (30)

Note that Eqs. 27 to 30 are exactly analogous to Eqs. (H&P) 6.1.5 to 6.1.8.

Finally Eq. 27 is substituted into Eqs. 21 to 23 to obtain the complete incremental relationships, which can be expressed in a fashion similar to that of Eq. (H&P) 6.1.10:

\[ \begin{cases} 
- \dot{\epsilon}_{ij} \\
- \dot{s} \\
- \dot{\chi}_{ij}(\eta) \\
\dot{\alpha}_{ij}(\eta) \\
\dot{\lambda}(\eta)
\end{cases} = \begin{bmatrix}
D_{ijkl}^{g,\sigma} & D_{ij}^{g,\theta}
\end{bmatrix}
\begin{bmatrix}
\Gamma_k
\end{bmatrix}
\begin{bmatrix}
\dot{\sigma}_{ij} \\
\dot{\theta}
\end{bmatrix}
\hspace{1cm} (31)

where

\[ D_{ijkl}^{g,\sigma} = \int \left( \frac{\partial^2 \hat{g}}{\partial \sigma_{ij} \partial \sigma_{kl}} + \frac{\partial^2 \hat{g}}{\partial \sigma_{ij} \partial \alpha_{mn}} \right) \hat{C}_{ijkl}^{g,\sigma} \Gamma(\eta) \kappa \eta \hspace{1cm} (32) \]

\[ D_{ij}^{g,\theta} = \int \left( \frac{\partial^2 \hat{g}}{\partial \sigma_{ij} \partial \theta} + \frac{\partial^2 \hat{g}}{\partial \alpha_{mn}} \hat{C}_{ij}^{g,\sigma} \right) \Gamma(\eta) \kappa \eta \hspace{1cm} (34) \]

\[ D_{kl}^{g,\theta} = \int \left( \frac{\partial^2 \hat{g}}{\partial \theta \partial \sigma_{kl}} + \frac{\partial^2 \hat{g}}{\partial \sigma_{ij} \partial \alpha_{mn}} \hat{C}_{ijkl}^{g,\sigma} \right) \Gamma(\eta) \kappa \eta \hspace{1cm} (33) \]

\[ D_{ij}^{g,\theta} = \int \left( \frac{\partial^2 \hat{g}}{\partial \theta^2} + \frac{\partial^2 \hat{g}}{\partial \sigma_{ij} \partial \alpha_{mn}} \hat{C}_{ij}^{g,\sigma} \left( \eta \right) \right) \Gamma(\eta) \kappa \eta \hspace{1cm} (35) \]

\[ \dot{D}_{ijkl}^{g,\sigma}(\eta) = \frac{\partial^2 \hat{g}}{\partial \sigma_{ij} \partial \alpha_{kl}} + \frac{\partial^2 \hat{g}}{\partial \sigma_{ij} \partial \sigma_{mn}} \hat{C}_{ijkl}^{g,\sigma}(\eta) \hspace{1cm} (36) \]

\[ \dot{D}_{kl}^{g,\theta}(\eta) = \frac{\partial^2 \hat{g}}{\partial \sigma_{ij} \partial \theta} + \frac{\partial^2 \hat{g}}{\partial \alpha_{mn}} \hat{C}_{ijkl}^{g,\sigma}(\eta) \hspace{1cm} (37) \]

\[ \dot{C}_{ijkl}^{g,\sigma}(\eta) = -\frac{\dot{A}_{kl}^{g,\sigma}(\eta)}{\hat{B}_{ij}^{g}(\eta)} \frac{\partial \hat{g}}{\partial \hat{\lambda}_{mn}} \hspace{1cm} (38) \]

\[ \dot{C}_{ij}^{g,\theta}(\eta) = -\frac{\dot{A}_{kl}^{g,\theta}(\eta)}{\hat{B}_{ij}^{g}(\eta)} \frac{\partial \hat{g}}{\partial \hat{\lambda}_{mn}} \hspace{1cm} (39) \]

Equations 31 to 39 are closely analogous to Eqs. (H&P) 6.1.10 to 6.1.16.
Thus we can see that the entire constitutive seponse of the material (expressed through the incremental stress-strain relationships and the evolution equations for the internal variables) can be derived from the original two thermodynamic functionals.

H&P discuss a number of cases in which constraints are imposed (for example on the rates of the internal variables). Constraints may also be necessary within this new formulation, but have not been addressed here.

CONCLUSIONS

In this paper we have generalised results previously obtained by H&P for plastic materials with a single tensorial internal variable to the case of multiple, and even infinite numbers of internal variables. The motivation is to allow the development of more sophisticated models, and in particular to achieve smooth transitions of stiffness. The case of an infinite number of internal variables involves replacing energy and dissipation functions by equivalent functionals. Whilst much of the formalism remains closely analogous to that developed by H&P, it has been necessary to introduce a number of new techniques. The purpose here has been to set out the formalism to be adopted: example applications will be the subject of separate publications.

REFERENCES


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<tr>
<td><strong>Typical yield function(al)</strong></td>
<td>$y^{g}(\sigma_{ij}, \alpha_{ij}, \theta, \chi_{ij}) = 0$</td>
<td>$y^{g}(\sigma_{ij}, \alpha_{ij}^{(1)}, ..., \alpha_{ij}^{(N)}, \theta, \chi_{ij}^{(n)}) = 0$</td>
<td>$\dot{y}^{g}(\sigma_{ij}, \dot{\alpha}<em>{ij}(\eta), \theta, \dot{\chi}</em>{ij}(\eta), \eta) = 0$</td>
</tr>
<tr>
<td><strong>Typical derivatives</strong></td>
<td>$\varepsilon_{ij} = -\frac{\partial g}{\partial \sigma_{ij}}$</td>
<td>$\varepsilon_{ij} = -\frac{\partial g}{\partial \sigma_{ij}}$</td>
<td>$\varepsilon_{ij} = -\frac{\partial g}{\partial \sigma_{ij}} = -\int_{\gamma}^{d^{g}} \frac{\partial \dot{g}}{\partial \sigma_{ij}} \Gamma(\eta) d\eta$</td>
</tr>
<tr>
<td></td>
<td>$\bar{\chi}<em>{ij} = -\frac{\partial g}{\partial \alpha</em>{ij}}$</td>
<td>$\bar{\chi}<em>{ij} = -\frac{\partial g}{\partial \alpha</em>{ij}^{(n)}}$</td>
<td>$\dot{\bar{\chi}}<em>{ij}(\eta) = -\frac{\partial \dot{g}}{\partial \dot{\alpha}</em>{ij}(\eta)}$</td>
</tr>
<tr>
<td></td>
<td>$s = -\frac{\partial g}{\partial \theta}$</td>
<td>$s = -\frac{\partial g}{\partial \theta}$</td>
<td>$s = -\frac{\partial g}{\partial \theta} = -\int_{\gamma}^{d^{g}} \frac{\partial \dot{g}}{\partial \theta} \Gamma(\eta) d\eta$</td>
</tr>
<tr>
<td><strong>Incremental response</strong></td>
<td>Eqs (H&amp;P) 6.1.10 to 6.1.16</td>
<td>Eqs 31 to 39</td>
<td></td>
</tr>
</tbody>
</table>

Table 1: Examples of comparisons between different formulations
APPENDICES

Appendix 1: Frechet differentials

In the derivation of material behaviour from functions, much use is made of the conventional partial derivative of a function with respect to a variable. When using functionals ("functions of functions") it is necessary to extend this concept to that of the derivative of a functional with respect to a function. This generalisation is achieved through the use of the Frechet derivative.

I(a) Definitions

In the classical calculus of variations, the variation of a functional \( f[\hat{u}] \) is defined in terms of a variation \( \delta \hat{u} \) of its argument function:

\[
\delta f[\hat{u}, \delta \hat{u}] = \lim_{\varepsilon \to 0} \frac{f[\hat{u} + \varepsilon \delta \hat{u}] - f[\hat{u}]}{\varepsilon}
\]  \hspace{1cm} (A1.1)

where \( \varepsilon \) is a scalar. A more precise statement defining \( \delta f \) is based on a choice of norm in the space of \( f \):

\[
\lim_{\varepsilon \to 0} \left\| \delta f[\hat{u}, \delta \hat{u}] - f[\hat{u} + \varepsilon \delta \hat{u}] - f[\hat{u}] \right\| = 0 \hspace{1cm} (A1.2)
\]

For sufficiently well behaved functionals \( f \), \( \delta f \) will be a linear functional of \( \delta \hat{u} \), so that \( \delta f[\hat{u}, \alpha \delta \hat{u}] = \alpha \delta f[\hat{u}, \delta \hat{u}] \), for all scalars \( \alpha \), and \( \delta f[\hat{u}, \delta \hat{u}_1 + \delta \hat{u}_2] = \delta f[\hat{u}, \delta \hat{u}_1] + \delta f[\hat{u}, \delta \hat{u}_2] \), for all \( \delta \hat{u}_1 \) and \( \delta \hat{u}_2 \). In this case, the functional \( \delta f \) may be presented as the inner product of a linear operator and the function \( \delta \hat{u} \):

\[
\delta f[\hat{u}, \delta \hat{u}] = f'[\hat{u}] \delta \hat{u} \hspace{1cm} (A1.3)
\]

where the linear operator \( f' \) (depending on function \( \hat{u} \)) is known as the Gateaux derivative of the functional \( f \). An alternative basic definition for the generalised derivative of \( f \) (the Frechet derivative) requires that \( f' \) be that linear operator satisfying

\[
\lim_{\| \delta \hat{u} \| \to 0} \frac{\| f[\hat{u} + \delta \hat{u}] - f[\hat{u}] - f'[\hat{u}] \delta \hat{u} \|}{\| \delta \hat{u} \|} = 0 \hspace{1cm} (A1.4)
\]

It can be shown that the Gateaux and Frechet definitions are equivalent when the linear operator \( f' \) is continuous in the function \( \hat{u} \), and in this paper \( f' \) is referred as the Frechet derivative. It is not essential to retain the variational notation in the definition of the Frechet derivative, therefore, a variation \( \delta \hat{u} \) can be replaced by any fixed \( \hat{v} \). In fact, when this variation is replaced by the differential \( d\hat{u} \), the resulting functional \( df[\hat{u}, d\hat{u}] = f'[\hat{u}] d\hat{u} \) will be referred to as Frechet differential. Frechet derivatives are utilized in this paper for definition of Legendre transformations of functionals, while the Frechet differentials are used in derivation of incremental response of material behaviour.

I(b) Selected results

Although the Frechet derivative is defined for general functionals, we are here interested principally in functionals of the form:
\[ f[\hat{u}] = \int_Y \hat{f}(\hat{u}(\eta), \eta) \Gamma(\eta) d\eta \]  

...(A1.5)

where \( Y \) is the domain of \( \eta \), and \( \hat{f} \) is a continuously differentiable function of the variable \( \hat{u} \), which is in turn a function of \( \eta \).

Then, according to definitions (A1.3 and A1.4), the Frechet differential of the functional (A1.5) is defined by:

\[ df[\hat{u}, d\hat{u}] = f'[\hat{u}] d\hat{u}(\eta) = \int_Y \frac{\partial \hat{f}(\hat{u}, \eta)}{\partial \hat{u}} d\hat{u}(\eta) \Gamma(\eta) d\eta \]  

...(A1.6)

Consider more general case, when \( f[\hat{u}_1, \ldots, \hat{u}_N] = \int_Y \hat{f}(\hat{u}_1(\eta), \ldots, \hat{u}_N(\eta), \eta) \Gamma(\eta) d\eta \), where \( \hat{f} \) is a continuously differentiable function of functional variables \( \hat{u}_i, \ i = 1, \ldots, N \).

When the variable \( \hat{u} \) in definitions (A1.3 and A1.4) is identified as the full \( N \)-dimensional space of functions \( \hat{u}_i(\eta) \), then the Frechet differential is given by:

\[ df[\hat{u}, d\hat{u}] = f'[\hat{u}] d\hat{u} = \int_Y \sum_{i=1}^{N} \frac{\partial \hat{f}(\hat{u}_1, \ldots, \hat{u}_N, \eta)}{\partial \hat{u}_i} d\hat{u}_i(\eta) \Gamma(\eta) d\eta \]  

...(A1.7)

For definition of partial Legendre transformations, the variable \( \hat{u} \) in definition (A1.3 and A1.4) is identified as the \( n \)-dimensional subspace of the full \( N \)-dimensional space of functions \( \hat{u}_i(\eta) \). In this case, the corresponding Frechet derivative is given by the following operator \( f' \), which is linear in any integrable functions \( \hat{v}_i(\eta) \):

\[ f'[\hat{u}] \hat{v} = \int_Y \sum_{i=0}^{n} \frac{\partial \hat{f}(\hat{u}_1, \ldots, \hat{u}_N, \eta)}{\partial \hat{u}_k} \hat{v}_i(\eta) \Gamma(\eta) d\eta \]  

...(A1.8)

**Appendix 2: Legendre Transformations of Functionals**

2(a) Functional of a single function

Consider a functional:

\[ f[\hat{u}] = \int_Y \hat{f}(\hat{u}(\eta), \eta) \Gamma(\eta) d\eta \]  

...(A2.1)

where \( Y \) is the domain of \( \eta \) and \( \hat{f} \) is a continuously differentiable function of a functional variable \( \hat{u} \).

If \( \hat{v}(\eta) = \frac{\partial \hat{f}(\hat{u}, \eta)}{\partial \hat{u}} \), then define the Legendre transform of the function \( \hat{f} \) as:

\[ \hat{g}(\hat{v}, \eta) = -\hat{v} \hat{u} + \hat{f}(\hat{u}, \eta) \]  

...(A2.2)
it follows from the standard properties of the transform that \( \hat{u}(\eta) = -\frac{\partial \hat{g}(\hat{v}, \eta)}{\partial \hat{v}}. \)

The functional defined by:

\[
g[\hat{v}] = \int_{Y} \hat{g}(\hat{v}(\eta), \eta) \Gamma(\eta) k\eta = -\int_{Y} \hat{v}(\eta) \hat{u}(\eta) \Gamma(\eta) k\eta + f[\hat{u}] \tag{A2.3}
\]

may then be considered as the Legendre transform of the original functional, and using definitions of Appendix 1, it can be confirmed that this definition satisfies the appropriate differential conditions.

2(b) Functional of multiple functions

A case of interest in the present work is a Legendre transform of a functional of the form:

\[
f[\hat{y}, \hat{u}] = \int_{Y} \hat{f}(\hat{y}(\eta), \hat{u}(\eta), \eta) \Gamma(\eta) k\eta \tag{A2.4}
\]

where \( \hat{f} \) is a continuously differentiable function of functions \( \hat{u} \) and \( \hat{y} \).

Denoting \( \hat{v}(\eta) = \frac{\partial \hat{f}(\hat{y}, \hat{u}, \eta)}{\partial \hat{u}} \), the Legendre transform of the function \( \hat{f} \) in function \( \hat{u} \) is defined as:

\[
\hat{g}(\hat{y}, \hat{v}, \eta) = -\hat{v} \hat{u} + \hat{f}(\hat{y}, \hat{u}, \eta) \tag{A2.5}
\]

From the standard properties of the transform it follows that

\[
\hat{u} = -\frac{\partial g(\hat{y}, \hat{v}, \eta)}{\partial \hat{v}} \tag{A2.6}
\]

\[
\frac{\partial \hat{g}(\hat{y}, \hat{v}, \eta)}{\partial \hat{y}} = \frac{\partial \hat{f}(\hat{y}, \hat{u}, \eta)}{\partial \hat{y}} \tag{A2.7}
\]

Then, the Legendre transformation of functional (A2.4) in function \( \hat{u} \), with function \( \hat{y} \) being a passive variable, is given by the functional

\[
g[\hat{y}, \hat{v}] = \int_{Y} \hat{g}(\hat{y}(\eta), \hat{v}(\eta), \eta) \Gamma(\eta) k\eta = -\int_{Y} \hat{v}(\eta) \hat{u}(\eta) \Gamma(\eta) k\eta + f[\hat{y}, \hat{u}] \tag{A2.8}
\]

and using definitions of Appendix 1, it can be confirmed that this definition satisfies the appropriate differential conditions.

In case when \( \hat{u} \) is not a function but a variable, denoted \( u \), all the above equations are valid, except that equation (A2.8) may be rewritten as:

\[
g[\hat{y}, v] = \int_{Y} \hat{g}(\hat{y}(\eta), v, \eta) \Gamma(\eta) k\eta = -vu + f[\hat{y}, u] \tag{A2.9}
\]

where:
\[ v = \int_Y \frac{\partial \hat{f}(\hat{y}, u, \eta)}{\partial u} \Gamma(\eta) \kappa \eta \]  

(A2.10)

In case when the function \( \hat{f} \) is a continuously differentiable function of \( \hat{u} \) (or variable \( u \)) and any finite number \( N \) of functions \( \hat{y}_i \), the same equations (A2.5 to A2.8) are still valid, except that equation (A2.7) unfolds into \( N \) equations:

\[ \frac{\partial \hat{g}(\hat{y}_1, \ldots, \hat{y}_N, \hat{v}, \eta)}{\partial \hat{y}_i} = \frac{\partial \hat{f}(\hat{y}_1, \ldots, \hat{y}_N, \hat{u}, \eta)}{\partial \hat{y}_i}, \quad i = 1, \ldots, N \]  

(A2.11)

2 (c) The singular transformation

An important case in rate-independent plasticity theory occurs when function \( \hat{f}(\hat{y}, \hat{u}, \eta) \) of functional (A2.4) is homogeneous of degree one in, say, \( \hat{u}(\eta) \):

\[ \hat{f}(\hat{y}, \lambda \hat{u}, \eta) = \lambda \hat{f}(\hat{y}, \hat{u}, \eta) \]  

(A2.12)

From Euler's theorem it follows that

\[ \hat{f}(\hat{y}, \hat{u}, \eta) = \frac{\partial \hat{f}(\hat{y}, \hat{u}, \eta)}{\partial \hat{u}} \hat{u}(\eta) = \hat{v}(\eta) \hat{u}(\eta) \]  

(A2.13)

Then the Legendre transformation of the function \( \hat{f}(\hat{y}, \hat{u}, \eta) \) with respect to \( \hat{u}(\eta) \), with other variables and functions being passive, is defined by equation (A2.5), so that after substitution of (A2.13) we obtain:

\[ \hat{g}(\hat{y}, \hat{v}, \eta) = -\hat{v} \hat{u} + \hat{f}(\hat{y}, \hat{u}, \eta) = 0 \]  

(A2.14)

The properties of this transformation are:

\[ \hat{u}(\eta) = \lambda(\eta) \frac{\partial \hat{g}(\hat{y}, \hat{v}, \eta)}{\partial \hat{v}} \]  

(A2.15)

\[ \frac{\partial \hat{f}(\hat{y}, \hat{u}, \eta)}{\partial \hat{y}} = \lambda(\eta) \frac{\partial \hat{g}(\hat{y}, \hat{v}, \eta)}{\partial \hat{v}} \]  

...(A2.16)

where \( \lambda(\eta) \) is an undetermined scalar, reflecting the non-unique nature of this singular transformation.

Then, the Legendre transformation of functional (A2.4) in function \( \hat{u} \), with function \( \hat{y} \) being a passive variable, is given by the functional:

\[ g[\hat{y}, \hat{v}] = \int_Y \hat{g}(\hat{y}(\eta), \hat{v}(\eta), \eta) \Gamma(\eta) \kappa \eta \]  

(A2.17)

and using definitions of Appendix 1, it can be confirmed that this definition satisfies the appropriate differential conditions.