

# Worst-Case Optimization of Failure Potentials

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In this document, we provide derivations for the constant coefficients of the von Mises, the Drucker-Prager, and the Bresler-Pister criteria, discussing how relevant strength parameters are characterized with mechanical testing. We further derive failure potentials for the latter criteria.

In a second part, we discuss implementation details on efficient gradient computations for our nested simulation, worst-case load, and design optimizations.

In the last section, we summarize additional validation examples for our worst-case load estimation.

## 1 FAILURE POTENTIALS

In the main text, we focused our discussion on the Bresler-Pister criterion. In this section, we will provide the reader with derivations of the constant coefficients of the von Mises, Drucker-Prager, and Bresler-Pister criteria. Coefficients are parameterized with uniaxial and biaxial tensile and compressive strength values. We will discuss how these parameters are estimated from mechanical testing data. Moreover, we will derive failure potentials for each criterion, enabling the formulation and optimization of stress objectives.

For the reader’s convenience, we herein include the table with stress quantities from the main text (see Tab. 1), where  $\sigma_m = \frac{1}{3}I_1$  is the mean or pure hydrostatic stress. The Haigh-Westergaard coordinates  $(\xi, \rho, \theta)$  for a stress point  $\sigma$  with principal stresses  $(\sigma_1, \sigma_2, \sigma_3)$  are

$$\xi = \frac{1}{\sqrt{3}}I_1 \quad \rho = \sqrt{2J_2} \quad \theta = \arccos\left(\frac{\sqrt{3}}{2} \frac{s_1}{\sqrt{J_2}}\right).$$

### 1.1 von Mises Criterion

The von Mises criterion has a single constant coefficient  $A$

$$h_{\text{VM}}(\xi, \rho, \theta) = \frac{1}{\sqrt{2}}\rho - A = \sqrt{J_2} - A = 0 \quad (1)$$

To derive an expression for the constant coefficient  $A$ , we perform an uniaxial tensile (or compression) test, resulting in an estimate of the uniaxial strength  $\sigma = \sigma_t = \sigma_c$  of the material. For an uniaxial test, the first principal stress  $\sigma_1$  equals  $\sigma$  at the point of failure, while the other two principal stresses  $\sigma_2$  and  $\sigma_3$  are zero. Plugged into invariants in Tab. 1, we can calculate the second invariant of the deviatoric stress ( $I_1 = \sigma$  and  $I_2 = 0$  imply  $J_2 = \frac{1}{3}\sigma^2$ ), resulting in the single-parameter coefficient

$$A(\sigma) = \sqrt{J_2} = \frac{1}{\sqrt{3}}\sigma.$$

To derive the corresponding failure potential, we multiply the strength parameter in  $A(\sigma)$  with a scale factor  $s$ . The failure potential is therefore

$$s_{\text{VM}}(\sigma) = \frac{\sqrt{J_2}}{A} \quad (2)$$

where we make use of the identity  $A(s\sigma) = sA(\sigma)$ .

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Table 1. Stress quantities.

Cauchy stress $\sigma$		deviatoric stress $\mathbf{s} = \sigma - \sigma_m \mathbf{I}$	
$(\sigma_1, \sigma_2, \sigma_3)$		$(s_1, s_2, s_3)$	
$I_1$	$= \text{tr}(\sigma)$ $= \sigma_1 + \sigma_2 + \sigma_3$	$J_1$	$= \text{tr}(\mathbf{s})$ $= s_1 + s_2 + s_3 = 0$
$I_2$	$= \frac{1}{2} [\text{tr}(\sigma)^2 + \text{tr}(\sigma^2)]$ $= \sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1$	$J_2$	$= \frac{1}{2} \text{tr}(\mathbf{s}^2) = \frac{1}{3}I_1^2 - I_2$ $= \frac{1}{2} (s_1^2 + s_2^2 + s_3^2)$
$I_3$	$= \det(\sigma)$ $= \sigma_1\sigma_2\sigma_3$	$J_3$	$= \det(\mathbf{s})$ $= s_1s_2s_3$

Note that the von Mises criterion is only valid for materials with insignificant differences in tensile and compressive strength. To identify its strength parameter  $\sigma$ , a tensile test with a standard bone-shaped specimen is sufficient, dividing the force at the point of failure by the specimen’s cross-sectional area. Alternatively, a compression test can be performed.

### 1.2 Drucker-Prager Criterion

The open cone shape of the failure surface of the Drucker-Prager criterion is defined implicitly as isosurface

$$h_{\text{DP}}(\xi, \rho, \theta) = \frac{1}{\sqrt{2}}\rho - A - \sqrt{3}B\xi = \sqrt{J_2} - A - BI_1 = 0. \quad (3)$$

To derive expressions for the two constant coefficients  $A$  and  $B$ , we perform uniaxial tensile and compression tests, resulting in strength values  $\sigma_t$  and  $\sigma_c$ . Under uniaxial tension, the principal stresses are  $\sigma_1 = \sigma_t, \sigma_2 = \sigma_3 = 0$  and relevant invariants simplify to  $I_1 = \sigma_t, I_2 = 0, J_2 = \frac{1}{3}\sigma_t^2$ , resulting in a first equation  $\frac{1}{\sqrt{3}}\sigma_t = A + B\sigma_t$  in the unknown coefficients. To derive a second equation, we look at a specimen’s behavior under uniaxial compression where the first principal stress flips its sign  $\sigma_1 = -\sigma_c$  while the other two remain zero  $\sigma_2 = \sigma_3 = 0$ . The relevant invariants are therefore  $I_1 = -\sigma_c, I_2 = 0$ , and  $J_2 = \frac{1}{3}(-\sigma_c)^2$ , resulting in the equation  $\frac{1}{\sqrt{3}}\sigma_c = A - B\sigma_c$ .

Solving the two equations for the two unknowns, we get expressions for the coefficients

$$A(\sigma_t, \sigma_c) = \frac{2}{\sqrt{3}} \frac{\sigma_t \sigma_c}{\sigma_t + \sigma_c} \quad \text{and} \quad B(\sigma_t, \sigma_c) = \frac{1}{\sqrt{3}} \frac{\sigma_t - \sigma_c}{\sigma_t + \sigma_c}.$$

Multiplying strength parameters in  $A(\sigma_t, \sigma_c)$  and  $B(\sigma_t, \sigma_c)$  with a scale factor  $s$ , we derive the corresponding failure potential

$$s_{\text{DP}}(\sigma) = \frac{\sqrt{J_2} - BI_1}{A} \quad (4)$$

where we make use of the identities  $A(s\sigma_t, s\sigma_c) = sA(\sigma_t, \sigma_c)$  and  $B(s\sigma_t, s\sigma_c) = B(\sigma_t, \sigma_c)$ .

### 1.3 Bresler-Pister Criterion

To derive expressions for the three coefficients of the Bresler-Pister criterion

$$h_{BP}(\xi, \rho, \theta) = \frac{1}{\sqrt{2}}\rho - A - \sqrt{3}B\xi - 3C\xi^2 = \sqrt{J_2} - A - BI_1 - CI_1^2 = 0 \quad (5)$$

the characterization of the material's uniaxial behavior is insufficient and an additional biaxial compression test is needed. If a test specimen breaks in uniaxial tension, or uniaxial or biaxial compression, the corresponding principal stresses  $(\sigma_1, \sigma_2, \sigma_3)$  are  $(\sigma_t, 0, 0)$ ,  $(-\sigma_c, 0, 0)$ , and  $(-\sigma_b, -\sigma_b, 0)$ , respectively, where  $\sigma_b$  is the biaxial compressive strength of the material. Plugging into expressions for invariants  $I_1, I_2$ , and  $J_2$ , we end up with a  $3 \times 3$ -equation system

$$\begin{bmatrix} 1 & \sigma_t & \sigma_t^2 \\ 1 & -\sigma_c & \sigma_c^2 \\ 1 & -2\sigma_b & 4\sigma_b^2 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} = \frac{1}{\sqrt{3}} \begin{bmatrix} \sigma_t \\ \sigma_c \\ \sigma_b \end{bmatrix}$$

that we can solve for the unknown coefficients

$$\begin{aligned} A(\sigma_t, \sigma_c, \sigma_b) &= \frac{1}{\sqrt{3}} \frac{\sigma_c \sigma_b \sigma_t (\sigma_t + 8\sigma_b - 3\sigma_c)}{(\sigma_c + \sigma_t)(2\sigma_b - \sigma_c)(2\sigma_b + \sigma_t)} \\ B(\sigma_t, \sigma_c, \sigma_b) &= \frac{1}{\sqrt{3}} \frac{(\sigma_c - \sigma_t)(\sigma_b \sigma_c + \sigma_b \sigma_t - \sigma_c \sigma_t - 4\sigma_b^2)}{(\sigma_c + \sigma_t)(2\sigma_b - \sigma_c)(2\sigma_b + \sigma_t)} \\ C(\sigma_t, \sigma_c, \sigma_b) &= \frac{1}{\sqrt{3}} \frac{3\sigma_b \sigma_t - \sigma_b \sigma_c - 2\sigma_c \sigma_t}{(\sigma_c + \sigma_t)(2\sigma_b - \sigma_c)(2\sigma_b + \sigma_t)}. \end{aligned}$$

We then use the identities

$$\begin{aligned} A(s\sigma_t, s\sigma_c, s\sigma_b) &= sA(\sigma_t, \sigma_c, \sigma_b) \\ B(s\sigma_t, s\sigma_c, s\sigma_b) &= B(\sigma_t, \sigma_c, \sigma_b) \\ C(s\sigma_t, s\sigma_c, s\sigma_b) &= \frac{1}{s}C(\sigma_t, \sigma_c, \sigma_b). \end{aligned}$$

for a uniform scaling factor  $s$  to derive the following quadratic equation from the Bresler-Pister criterion

$$\sqrt{J_2} = sA + BI_1 + \frac{1}{s}CI_1^2$$

whose positive solution provides us with a failure potential

$$s_{BP}(\sigma) = \frac{\sqrt{J_2} - BI_1 + \sqrt{(B^2 - 4AC)I_1^2 - 2BI_1\sqrt{J_2} + J_2}}{2A}. \quad (6)$$

## 2 EFFICIENT WORST-CASE OPTIMIZATION

In this section, we explain how we apply the adjoint method to efficiently compute analytical gradients of our worst-case load and design optimization efficiently.

### 2.1 Worst-Case Load Estimation

To compute the gradient for our worst-case load estimation

$$g_{fail}(\mathbf{p}) = -\frac{\partial f_{fail}(\mathbf{x})}{\partial \mathbf{x}} \frac{d\mathbf{x}(\mathbf{p})}{d\mathbf{p}} + \frac{\partial R(\mathbf{p})}{\partial \mathbf{p}},$$

we treat the first-order optimality constraints implicitly and compute the Jacobian of the deformed configuration with respect to the parameters  $\mathbf{p}$

$$\frac{d\mathbf{x}(\mathbf{p})}{d\mathbf{p}} = -H_{sim}^{-1}(\mathbf{x}) \frac{\partial g_{sim}(\mathbf{l}, \mathbf{x})}{\partial \mathbf{l}} \frac{\partial \mathbf{l}(\mathbf{p})}{\partial \mathbf{p}}.$$

with the help of the implicit function theorem. However, in this particular form, the computation of the Jacobian would require  $3n$  system solves where  $n$  is the number of nodes (including the additional degrees of freedom for enriched elements). For efficient computations, we reorder multiplications, applying the *adjoint method*. To this end, we first insert Eq. (7) into Eq. (7),

$$g_{fail}(\mathbf{p}) = \frac{\partial f_{fail}(\mathbf{x})}{\partial \mathbf{x}} H_{sim}^{-1}(\mathbf{x}) \frac{\partial g_{sim}(\mathbf{l}, \mathbf{x})}{\partial \mathbf{l}} \frac{\partial \mathbf{l}(\mathbf{p})}{\partial \mathbf{p}} + \frac{\partial R(\mathbf{p})}{\partial \mathbf{p}}.$$

We then set the first two terms equal to  $\lambda^T$ , resulting in the adjoint system

$$H_{sim}(\mathbf{x})\lambda = \left( \frac{\partial f_{fail}(\mathbf{x})}{\partial \mathbf{x}} \right)^T. \quad (7)$$

By solving a *single* system, we can then form the gradient

$$g_{fail}(\mathbf{p}) = \lambda^T \frac{\partial g_{sim}(\mathbf{l}, \mathbf{x})}{\partial \mathbf{l}} \frac{\partial \mathbf{l}(\mathbf{p})}{\partial \mathbf{p}} + \frac{\partial R(\mathbf{p})}{\partial \mathbf{p}}. \quad (8)$$

### 2.2 Design Optimization

To compute the analytical gradient of our design objective (compare with main text)

$$g_{design}(\phi) = \frac{\partial f_{design}(\phi, \mathbf{x})}{\partial \phi} + \frac{\partial f_{design}(\phi, \mathbf{x})}{\partial \mathbf{x}} \frac{d\mathbf{x}(\phi)}{d\phi},$$

we follow the same recipe, enforcing the first-optimality of our simulation and worst-case load estimation implicitly

$$\begin{bmatrix} \frac{d\mathbf{p}(\phi)}{d\phi} \\ \frac{d\mathbf{x}(\phi)}{d\phi} \end{bmatrix} = - \begin{bmatrix} H_{fail}(\phi, \mathbf{p}, \mathbf{x}) & \frac{g_{fail}(\phi, \mathbf{p}, \mathbf{x})}{\partial \mathbf{x}} \\ \frac{\partial g_{sim}(\phi, \mathbf{l}, \mathbf{x})}{\partial \mathbf{l}} \frac{\partial \mathbf{l}(\mathbf{p})}{\partial \mathbf{p}} & H_{sim}(\phi, \mathbf{x}) \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial g_{fail}(\phi, \mathbf{p}, \mathbf{x})}{\partial \phi} \\ \frac{\partial g_{sim}(\phi, \mathbf{l}, \mathbf{x})}{\partial \phi} \end{bmatrix}.$$

For efficient computation, we again turn to the adjoint method. Inserting Eq. (9) into Eq. (9), we arrive at

$$g_{design}(\phi) = \frac{\partial f_{design}(\phi, \mathbf{x})}{\partial \phi} - \left[ \left( \frac{\partial f_{design}(\phi, \mathbf{x})}{\partial \mathbf{x}} \right)^T \right] \begin{bmatrix} H_{fail}(\phi, \mathbf{p}, \mathbf{x}) & \frac{g_{fail}(\phi, \mathbf{p}, \mathbf{x})}{\partial \mathbf{x}} \\ \frac{\partial g_{sim}(\phi, \mathbf{l}, \mathbf{x})}{\partial \mathbf{l}} \frac{\partial \mathbf{l}(\mathbf{p})}{\partial \mathbf{p}} & H_{sim}(\phi, \mathbf{x}) \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial g_{fail}(\phi, \mathbf{p}, \mathbf{x})}{\partial \phi} \\ \frac{\partial g_{sim}(\phi, \mathbf{l}, \mathbf{x})}{\partial \phi} \end{bmatrix},$$

setting up the adjoint equation

$$\begin{bmatrix} H_{fail}(\phi, \mathbf{p}, \mathbf{x}) & \frac{g_{fail}(\phi, \mathbf{p}, \mathbf{x})}{\partial \mathbf{x}} \\ \frac{\partial g_{sim}(\phi, \mathbf{l}, \mathbf{x})}{\partial \mathbf{l}} \frac{\partial \mathbf{l}(\mathbf{p})}{\partial \mathbf{p}} & H_{sim}(\phi, \mathbf{x}) \end{bmatrix}^T \begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \left( \frac{\partial f_{design}(\phi, \mathbf{x})}{\partial \mathbf{x}} \right)^T \end{bmatrix}.$$

We then use its solution  $\begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix}$  to compute the final gradient

$$g_{design}(\phi) = \frac{\partial f_{design}(\phi, \mathbf{x})}{\partial \phi} - \begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix}^T \begin{bmatrix} \frac{\partial g_{fail}(\phi, \mathbf{p}, \mathbf{x})}{\partial \phi} \\ \frac{\partial g_{sim}(\phi, \mathbf{l}, \mathbf{x})}{\partial \phi} \end{bmatrix}.$$

## 3 VALIDATION: WORST-CASE LOAD ESTIMATION

We further validate our worst-case optimization with a bar and an I-beam example attached to a wall at one end (see Fig. 1). For both examples, we define the top part of the models as the regions where the worst-case loads can act. After sampling 10 initial load locations and picking the best starting point, the optimization for the worst-case loads converges to a load location at the free end of the models, matching the globally optimal worst-case load position.

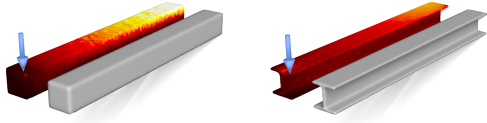


Fig. 1. **Worst-Case Loads** For a bar and an I-beam, we can predict where worst-case loads appear. Our worst-case optimization correctly identifies the optimal force locations at the free end of the bar and beam.