Microscopic Simulation of Solid State Sintering Regarding Irregularly Shaped Powder Particles

Max Weiner

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Classic Formulation

$$\mathcal{D}(\boldsymbol{X}, \boldsymbol{x}, \dot{\boldsymbol{x}}) = \frac{\partial G(\boldsymbol{X}, \boldsymbol{x})}{\partial \boldsymbol{x}} \cdot \dot{\boldsymbol{x}} \to \max_{\dot{\boldsymbol{x}}} \tag{1.1a}$$

$$\mathcal{D}(\boldsymbol{X}, \boldsymbol{x}, \dot{\boldsymbol{x}}) - \mathcal{Q}(\boldsymbol{X}, \boldsymbol{x}, \dot{\boldsymbol{x}}) = 0 \tag{1.1b}$$

$$\mathcal{L} = \mathcal{D}(\boldsymbol{X}, \boldsymbol{x}, \dot{\boldsymbol{x}}) + \lambda \left(\mathcal{D}(\boldsymbol{X}, \boldsymbol{x}, \dot{\boldsymbol{x}}) - \mathcal{Q}(\boldsymbol{X}, \boldsymbol{x}, \dot{\boldsymbol{x}})\right) \tag{1.2}$$

$$\boldsymbol{\mathcal{L}}_{\dot{\boldsymbol{x}}} = (1 + \lambda) \frac{\partial G(\boldsymbol{X}, \boldsymbol{x})}{\partial \boldsymbol{x}} - \lambda \frac{\partial \mathcal{Q}(\boldsymbol{X}, \boldsymbol{x}, \dot{\boldsymbol{x}})}{\partial \dot{\boldsymbol{x}}} \tag{1.3a}$$

$$\mathcal{L}_{\lambda} = \mathcal{D}(\boldsymbol{X}, \boldsymbol{x}, \dot{\boldsymbol{x}}) - \mathcal{Q}(\boldsymbol{X}, \boldsymbol{x}, \dot{\boldsymbol{x}}) \tag{1.3b}$$

Generalized Formulation

Acc. to **Hackl2020**

$$\mathcal{D}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}}) = \frac{\partial G(\boldsymbol{X},\boldsymbol{x})}{\partial \boldsymbol{x}} \cdot \dot{\boldsymbol{x}} \to \max_{\dot{\boldsymbol{x}}} \tag{1.4a}$$

$$\mathcal{D}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}}) - \mathcal{Q}(\boldsymbol{X},\boldsymbol{x},\boldsymbol{j}) = 0 \tag{1.4b}$$

$$\boldsymbol{f}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{j}) = 0 \tag{1.4c}$$

$$\boldsymbol{g}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{j}) = 0 \tag{1.4d}$$

$$\mathcal{L} = \mathcal{D}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}}) + \lambda_1 \left(\mathcal{D}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}}) - \mathcal{Q}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}})\right) + \boldsymbol{\lambda_2} \cdot \boldsymbol{f}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{j}) + \boldsymbol{\lambda_3} \cdot \boldsymbol{g}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{j}) \tag{1.5}$$

$$\boldsymbol{\mathcal{L}}_{\dot{\boldsymbol{x}}} = (1+\lambda_1)\,\frac{\partial G(\boldsymbol{X},\boldsymbol{x})}{\partial \boldsymbol{x}} - \lambda_1 \frac{\partial \mathcal{Q}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}})}{\partial \dot{\boldsymbol{x}}} + \boldsymbol{\lambda_2} \frac{\partial \boldsymbol{f}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{j})}{\partial \dot{\boldsymbol{x}}} + \boldsymbol{\lambda_3} \frac{\partial \boldsymbol{g}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{j})}{\partial \dot{\boldsymbol{x}}} \tag{1.6a}$$

$$\mathcal{L}_{\lambda_1} = \mathcal{D}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}}) - \mathcal{Q}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}}) \tag{1.6b}$$

$$\boldsymbol{\mathcal{L}}_{\boldsymbol{\lambda_2}} = \boldsymbol{f}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{j}) \tag{1.6c}$$

$$\boldsymbol{\mathcal{L}}_{\boldsymbol{\lambda_3}} = \boldsymbol{g}(\boldsymbol{X},\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{j}) \tag{1.6d}$$

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