

Supplementary Information

Non-isothermal phase-field modeling of heat-melt-microstructure coupled processes during powder bed fusion

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Supplementary Note 1: Derivation of kinetic equations

Here we present the derivation of the kinetic system for OPs, melt flow dynamic as well as transient heat transfer, which is based on the works in [1–7]. We firstly construct the total energy $\bar{\mathcal{E}}$ for the whole system as the summation of the internal energy $\mathcal{E}$ and the kinetic energy $\mathcal{K}$

$$\begin{aligned}\bar{\mathcal{E}} &= \mathcal{E}(\rho, \phi, \{\eta_j\}) + \mathcal{K}(\rho, \mathbf{u}) \\ &= \int_{\Omega} \left[e(\rho, \phi, \{\eta_j\}) + \frac{1}{2} \varrho(\rho) |\mathbf{u}|^2 \right] d\Omega.\end{aligned}\tag{S1}$$

Notice that the density ϱ is only a function of the conserved OP ρ assuming the density difference between liquid and solid is negligible. According to the first law of the thermodynamics, temporal variation of the total energy of the subdomain Ω within a close boundary Γ should obey

$$\frac{d\bar{\mathcal{E}}}{dt} = \int_{\Omega} \varrho \mathbf{b} \cdot \mathbf{u} d\Omega + \int_{\Gamma} (\boldsymbol{\sigma} \cdot \mathbf{u}) \cdot \mathbf{n} d\Gamma - \int_{\Gamma} (\mathbf{j}_e + \mathbf{j}_q) \cdot \mathbf{n} d\Gamma,\tag{S2a}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor of the system which is assumed to be symmetric, $\mathbf{b}$ is the body force, $\mathbf{j}_e$ is the thermal flux due to the heat transfer, and $\mathbf{j}_q$ is the power flux due to the external energy input, e.g. laser or electron beam. Using the Reynolds transfer theorem and Gaussian theorem, the left-hand side of Eq. (S2a) becomes

$$\begin{aligned}\frac{d\bar{\mathcal{E}}}{dt} &= \int_{\Omega} \dot{\bar{\mathcal{E}}} d\Omega + \int_{\Gamma} \bar{\mathcal{E}} \mathbf{u} \cdot \mathbf{n} d\Gamma = \int_{\Omega} [\dot{\bar{\mathcal{E}}} + \nabla \cdot (\bar{\mathcal{E}} \mathbf{u})] d\Omega \\ &= \int_{\Omega} \left[\frac{D\bar{\mathcal{E}}}{Dt} + \bar{\mathcal{E}} \nabla \cdot \mathbf{u} \right] d\Omega,\end{aligned}\tag{S2b}$$

where the total energy density $\bar{\mathcal{E}}(\rho, \phi, \{\eta_j\}, \mathbf{u}) = e(\rho, \phi, \{\eta_j\}) + \frac{1}{2} \varrho(\rho) |\mathbf{u}|^2$. Notice that due to the coupling with velocity, we use the material derivative $D(\cdot)/Dt = (\dot{\cdot}) + (\mathbf{u} \cdot \nabla)(\cdot)$ to present the temporal variation with $\mathbf{u}$ as the flow velocity. After expanding $d\bar{\mathcal{E}}/dt$ and neglect the effect of density variation of flow, we combine Eqs. (S2a) and (S2b), yield

$$\frac{De}{Dt} = \varrho \mathbf{b} \cdot \mathbf{u} + \nabla \cdot (\boldsymbol{\sigma} \cdot \mathbf{u}) - \varrho \mathbf{u} \cdot \frac{D\mathbf{u}}{Dt} - \frac{1}{2} \varrho |\mathbf{u}|^2 \nabla \cdot \mathbf{u} - \nabla \cdot (\mathbf{j}_e + \mathbf{j}_q).\tag{S3}$$

In this case, we assume that the fluid system obeys the INS equations,

$$\nabla \cdot \mathbf{u} = 0,\tag{S4a}$$

$$\varrho \frac{D\mathbf{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{b},\tag{S4b}$$

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where $\boldsymbol{\sigma}$ is the Cauchy stress tensor and $\mathbf{b}$ the body force. The local energy conservation inside a subdomain Ω with a close boundary Γ can be formulated as follows after expanding Eq. (S3) and considering the incompressible condition in Eq. (S4a)

$$\frac{De}{Dt} = \boldsymbol{\sigma} : \nabla \mathbf{u} - \nabla \cdot \mathbf{j}_e - \nabla \cdot \mathbf{j}_q = \boldsymbol{\sigma} : \nabla \mathbf{u} - \nabla \cdot \mathbf{j}_e + q_v, \quad (\text{S5})$$

where $\mathbf{j}_e$ is the thermal flux due to the heat transfer, and $\mathbf{j}_q$ is the power flux due to the external energy input, i.e. the laser beam or electron beam. In most researches, the thermal effect due to the external energy input is also equivalently treated as an internal heat source q_v moving with the scan speed $\mathbf{v}$ by replacing $-\nabla \cdot \mathbf{j}_q$ with a non-negative function q_v [8–11].

As for the mass conservation, we have

$$\dot{\rho} + \nabla \cdot (\rho \mathbf{u}) = -\nabla \cdot \mathbf{j}_\rho, \quad (\text{S6a})$$

where $\mathbf{j}_\rho$ indicates the mass transfer other than melt flow (here we treat it as diffusion dominant). Due to the incompressible condition in Eq. (S4a), $\nabla \cdot (\rho \mathbf{u}) = \nabla \rho : \mathbf{u}$. Thus, we can rewrite Eq. (S6a) as the material derivative form as

$$\frac{D\rho}{Dt} = -\nabla \cdot \mathbf{j}_\rho, \quad (\text{S6b})$$

Next, according to the second law of thermodynamics, the total production of the entropy should always be non-negative [4, 12]. For the subdomain Ω and its close boundary Γ , the production rate of the entropy can be formulate as

$$\frac{d\mathcal{S}}{dt} + \int_\Gamma \mathbf{j}_s \cdot \mathbf{n} d\Gamma \geq 0. \quad (\text{S7})$$

The temporal variation of the entropy $d\mathcal{S}/dt$ is calculated as

$$\begin{aligned} \frac{d\mathcal{S}}{dt} = \int_\Omega & \left[\frac{\partial s}{\partial e} \frac{De}{Dt} + \frac{\partial s}{\partial \rho} \frac{D\rho}{Dt} + \frac{\partial s}{\partial \phi} \frac{D\phi}{Dt} + \sum_j \frac{\partial s}{\partial \eta_j} \frac{D\eta_j}{Dt} \right. \\ & \left. + \frac{\partial s}{\partial \nabla \rho} \frac{D\nabla \rho}{Dt} + \frac{\partial s}{\partial \nabla \phi} \frac{D\nabla \phi}{Dt} + \sum_j \frac{\partial s}{\partial \nabla \eta_j} \frac{D\nabla \eta_j}{Dt} \right] d\Omega. \end{aligned} \quad (\text{S8a})$$

Notice that $D\nabla(\cdot)/Dt = \nabla[D(\cdot)/Dt] - \nabla \mathbf{u} \cdot \nabla(\cdot)$. After performing integration-by-parts on resulting $\nabla[D(\cdot)/Dt]$, we obtain

$$\begin{aligned} \frac{d\mathcal{S}}{dt} = \int_\Omega & \left[\frac{\delta \mathcal{S}}{\delta e} \frac{De}{Dt} + \frac{\delta \mathcal{S}}{\delta \rho} \frac{D\rho}{Dt} + \frac{\delta \mathcal{S}}{\delta \phi} \frac{D\phi}{Dt} + \sum_j \frac{\delta \mathcal{S}}{\delta \eta_j} \frac{D\eta_j}{Dt} \right. \\ & \left. - \frac{\partial s}{\partial \nabla \rho} \otimes \nabla \rho : \nabla \mathbf{u} - \frac{\partial s}{\partial \nabla \phi} \otimes \nabla \phi : \nabla \mathbf{u} - \sum_j \frac{\partial s}{\partial \nabla \eta_j} \otimes \nabla \eta_j : \nabla \mathbf{u} \right] d\Omega \\ & + \int_\Gamma \left[\frac{D\rho}{Dt} \frac{\partial s}{\partial \nabla \rho} + \frac{D\phi}{Dt} \frac{\partial s}{\partial \nabla \phi} + \sum_j \frac{D\eta_j}{Dt} \frac{\partial s}{\partial \nabla \eta_j} \right] \cdot \hat{\mathbf{n}} d\Gamma, \end{aligned} \quad (\text{S8b})$$

The surface integration is known as the entropy flux due to changes in the diffusive interfaces (a.k.a. gradient terms) of order parameters at the boundary Γ [12, 13]. Then the total entropy flux $\mathbf{j}_s$ in Eq. (S7) can be simply formulated as the combination of contributions from $\mathbf{j}_{ht}$ and $\mathbf{j}_\rho$ as well as the compensation from the interface term, i.e.

$$\mathbf{j}_s = \frac{\delta \mathcal{S}}{\delta e} \mathbf{j}_e + \frac{\delta \mathcal{S}}{\delta \rho} \mathbf{j}_\rho + \mathbf{j}_s^{\text{grad}}. \quad (\text{S9})$$

with

$$\mathbf{j}_s^{\text{grad}} = - \left(\frac{D\rho}{Dt} \frac{\partial s}{\partial \nabla \rho} + \frac{D\phi}{Dt} \frac{\partial s}{\partial \nabla \phi} + \sum_j \frac{D\eta_j}{Dt} \frac{\partial s}{\partial \nabla \eta_j} \right).$$

Substituting Eqs. (S5), (S6b) and (S9) into Eq. (S7) and performing integration-by-parts on certain terms, we obtain

$$\int_{\Omega} \left[\frac{\delta \mathcal{S}}{\delta e} q_{\mathbf{v}} + \nabla \frac{\delta \mathcal{S}}{\delta e} \cdot \mathbf{j}_e + \nabla \frac{\delta \mathcal{S}}{\delta \rho} \cdot \mathbf{j}_{\rho} + \frac{\delta \mathcal{S}}{\delta \phi} \frac{D\phi}{Dt} + \sum_j \frac{\delta \mathcal{S}}{\delta \eta_j} \frac{D\eta_j}{Dt} + \frac{\delta \mathcal{S}}{\delta e} \boldsymbol{\sigma} : \nabla \mathbf{u} - \frac{\partial s}{\partial \nabla \rho} \otimes \nabla \rho : \nabla \mathbf{u} - \frac{\partial s}{\partial \nabla \phi} \otimes \nabla \phi : \nabla \mathbf{u} - \sum_j \frac{\partial s}{\partial \nabla \eta_j} \otimes \nabla \eta_j : \nabla \mathbf{u} \right] d\Omega \geq 0. \quad (\text{S10})$$

Since the equivalent internal heat source $q_{\mathbf{v}}$ is already non-negative, a non-negative entropy production can be thereby guaranteed by taking the following relations into account,

$$\mathbf{j}_e = \hat{\mathbf{K}} \cdot \nabla \frac{\delta \mathcal{S}}{\delta e} = -\hat{\mathbf{K}} \cdot \frac{1}{T^2} \nabla T, \quad (\text{S11a})$$

$$\mathbf{j}_{\rho} = \hat{\mathbf{M}} \cdot \nabla \frac{\delta \mathcal{S}}{\delta \rho} = - \left[\frac{1}{T} \hat{\mathbf{M}} \cdot \nabla \frac{\delta \mathcal{F}}{\delta \rho} + \frac{1}{T} \hat{\mathbf{M}} \cdot \left(-\frac{\delta \mathcal{F}}{\delta \rho} \frac{\nabla T}{T} \right) \right], \quad (\text{S11b})$$

$$\frac{D\phi}{Dt} = \hat{L}_{\phi} \frac{\delta \mathcal{S}}{\delta \phi} = \hat{L}_{\phi} \left(-\frac{1}{T} \frac{\delta \mathcal{F}}{\delta \phi} \right), \quad (\text{S11c})$$

$$\frac{D\eta_j}{Dt} = \hat{L}_{\eta} \frac{\delta \mathcal{S}}{\delta \eta_j} = \hat{L}_{\eta} \left(-\frac{1}{T} \frac{\delta \mathcal{F}}{\delta \eta_j} \right), \quad (\text{S11d})$$

$$\frac{\delta \mathcal{S}}{\delta e} \boldsymbol{\sigma} : \nabla \mathbf{u} - \frac{\partial s}{\partial \nabla \rho} \otimes \nabla \rho : \nabla \mathbf{u} - \frac{\partial s}{\partial \nabla \phi} \otimes \nabla \phi : \nabla \mathbf{u} - \sum_j \frac{\partial s}{\partial \nabla \eta_j} \otimes \nabla \eta_j : \nabla \mathbf{u} \geq 0, \quad (\text{S11e})$$

with

$$\frac{\delta \mathcal{S}}{\delta \rho} = -\frac{1}{T} \frac{\delta \mathcal{F}}{\delta \rho}, \quad \frac{\delta \mathcal{S}}{\delta \phi} = -\frac{1}{T} \frac{\delta \mathcal{F}}{\delta \phi}, \quad \frac{\delta \mathcal{S}}{\delta \eta_j} = -\frac{1}{T} \frac{\delta \mathcal{F}}{\delta \eta_j}, \quad \frac{\delta \mathcal{S}}{\delta e} = \frac{1}{T},$$

and

$$\frac{\partial s}{\partial \nabla \rho} = -\kappa_{\rho} \nabla \rho - \kappa_{\phi} (\nabla \rho - \nabla \phi), \quad \frac{\partial s}{\partial \nabla \phi} = -\kappa_{\phi} \nabla \phi + \kappa_{\phi} (\nabla \rho - \nabla \phi), \quad \frac{\partial s}{\partial \nabla \eta_j} = -\kappa_{\eta} \nabla \eta_j.$$

Notice that $\hat{\mathbf{K}}$ and $\hat{\mathbf{M}}$ are positively defined tensors while $\hat{L}_{\phi}$, $\hat{L}_{\eta}$ and $\hat{V}$ are positive scalars. Up to this step, it is quite clear for Eq. (S11a)–(S11d) to have proper formulations, whereas the constitutive equation for the Cauchy stress tensor $\boldsymbol{\sigma}$ still needs to be determined to satisfy the inequality shown in Eq. (S11e) satisfied. We firstly rearrange Eq. (S11e) after substituting $\delta \mathcal{S}/\delta e$, $\partial s/\partial \nabla \rho$, $\partial s/\partial \nabla \phi$ and $\partial s/\partial \nabla \eta_j$ as

$$\left[\frac{1}{T} \boldsymbol{\sigma} + \kappa_{\rho} \nabla \rho \otimes \nabla \rho + \kappa_{\phi} \nabla \phi \otimes \nabla \phi + \kappa_{\phi} (\nabla \rho - \nabla \phi) \otimes (\nabla \rho - \nabla \phi) + \kappa_{\eta} \sum_j \nabla \eta_j \otimes \nabla \eta_j \right] : \nabla \mathbf{u} \geq 0. \quad (\text{S12})$$

Consider the following splitting without loss of generality

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}' - p\mathbf{I} \quad \text{with} \quad \boldsymbol{\sigma}' = \boldsymbol{\sigma} + p\mathbf{I}, \quad (\text{S13a})$$

$$\nabla \mathbf{u} = \boldsymbol{\varsigma} + \boldsymbol{\varsigma}' \quad \text{with} \quad \boldsymbol{\varsigma} = \frac{1}{2} [\nabla \mathbf{u} + (\nabla \mathbf{u})^T], \quad \boldsymbol{\varsigma}' = \frac{1}{2} [\nabla \mathbf{u} - (\nabla \mathbf{u})^T], \quad (\text{S13b})$$

where $\mathbf{I}$ is the identity tensor, p is a scalar, and notation $(\cdot)^T$ represents the transpose. Substituting Eq. (S13a) and (S13b) along with the incompressible condition in Eq. (S4a) into the term $\boldsymbol{\sigma} : \nabla \mathbf{u}$, yields

$$\begin{aligned} \boldsymbol{\sigma} : \nabla \mathbf{u} &= \boldsymbol{\sigma} : (\boldsymbol{\varsigma} + \boldsymbol{\varsigma}') = \boldsymbol{\sigma} : \boldsymbol{\varsigma} \\ &= (\boldsymbol{\sigma}' - p\mathbf{I}) : \boldsymbol{\varsigma} = \boldsymbol{\sigma}' : \boldsymbol{\varsigma}. \end{aligned} \quad (\text{S14a})$$

Since κ_ρ , κ_ϕ and κ_η are all constants, it is anticipated that $\kappa_\rho \nabla \rho \otimes \nabla \rho$, $\kappa_\phi \nabla \phi \otimes \nabla \phi$, $\kappa_\phi (\nabla \rho - \nabla \phi) \otimes (\nabla \rho - \nabla \phi)$ and $\kappa_\eta \nabla \eta_j \otimes \nabla \eta_j$ are all symmetric, thus

$$\begin{aligned}\kappa_\rho \nabla \rho \otimes \nabla \rho : \nabla \mathbf{u} &= \kappa_\rho \nabla \rho \otimes \nabla \rho : \boldsymbol{\varsigma}, \\ \kappa_\phi \nabla \phi \otimes \nabla \phi : \nabla \mathbf{u} &= \kappa_\phi \nabla \phi \otimes \nabla \phi : \boldsymbol{\varsigma}, \\ \kappa_\phi (\nabla \rho - \nabla \phi) \otimes (\nabla \rho - \nabla \phi) : \nabla \mathbf{u} &= \kappa_\phi (\nabla \rho - \nabla \phi) \otimes (\nabla \rho - \nabla \phi) : \boldsymbol{\varsigma}, \\ \kappa_\eta \nabla \eta_j \otimes \nabla \eta_j : \nabla \mathbf{u} &= \kappa_\eta \nabla \eta_j \otimes \nabla \eta_j : \boldsymbol{\varsigma}.\end{aligned}\tag{S14b}$$

Then we rearrange Eq. (S12) as

$$\left[\frac{1}{T} \boldsymbol{\sigma}' + \kappa_\rho \nabla \rho \otimes \nabla \rho + \kappa_\phi \nabla \phi \otimes \nabla \phi + \kappa_\phi (\nabla \rho - \nabla \phi) \otimes (\nabla \rho - \nabla \phi) + \kappa_\eta \sum_j \nabla \eta_j \otimes \nabla \eta_j \right] : \boldsymbol{\varsigma} \geq 0. \tag{S15}$$

As a consequence, we can guarantee the satisfaction of the inequality into Eq. (S15) by taking

$$\frac{1}{T} \boldsymbol{\sigma}' + \kappa_\rho \nabla \rho \otimes \nabla \rho + \kappa_\phi \nabla \phi \otimes \nabla \phi + \kappa_\phi (\nabla \rho - \nabla \phi) \otimes (\nabla \rho - \nabla \phi) + \kappa_\eta \sum_j \nabla \eta_j \otimes \nabla \eta_j = \hat{V} \boldsymbol{\varsigma}, \tag{S16}$$

where $\hat{V}$ is a positive constant (or function). If we adopt a new positive constant/function $\nu = \hat{V}T/2$, we obtain the constitutive equation of $\boldsymbol{\sigma}$ by substituting Eq. (S16) back to (S13a)

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\nu\boldsymbol{\varsigma} - T\kappa_\rho \nabla \rho \otimes \nabla \rho - T\kappa_\phi \nabla \phi \otimes \nabla \phi - T\kappa_\phi (\nabla \rho - \nabla \phi) \otimes (\nabla \rho - \nabla \phi) - T\kappa_\eta \sum_j \nabla \eta_j \otimes \nabla \eta_j. \tag{S17}$$

Here p is the hydrostatic stress and $\boldsymbol{\varsigma} = \frac{1}{2} [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]$ as the deviator. ν also adopts its physical meaning as the dynamic viscosity. After substituting Eq. (S17) back to (S4a) and (S4b) and combine all terms including gradients of OPs into a tensor $\boldsymbol{\sigma}_K$, we obtain the kinetic equations for the melting region

$$\nabla \cdot \mathbf{u} = 0, \tag{S18a}$$

$$\varrho \frac{d\mathbf{u}}{dt} = -\nabla p + \nu \nabla^2 \mathbf{u} - \nabla \cdot \boldsymbol{\sigma}_K + \mathbf{b}, \tag{S18b}$$

with

$$\boldsymbol{\sigma}_K = T\kappa_\rho \nabla \rho \otimes \nabla \rho + T\kappa_\phi \nabla \phi \otimes \nabla \phi + T\kappa_\phi (\nabla \rho - \nabla \phi) \otimes (\nabla \rho - \nabla \phi) + T\kappa_\eta \sum_j \nabla \eta_j \otimes \nabla \eta_j.$$

Here this tensor $\boldsymbol{\sigma}_K$ is known as Korteweg stress tensor, which reflects the effects of the interface tensions on the fluids [14, 15]. We then adopt new tensors $\mathbf{k} = \hat{\mathbf{K}}/T^2$, $\mathbf{M} = \hat{\mathbf{M}}/T$ and scalar $L_\phi = \hat{L}_\phi/T$ and $L_\eta = \hat{L}_\eta/T$, and substitute Eqs. (S11a), (S11b) and (S11e) back to Eqs. (S5), (S6b) and (S4b), respectively. Eventually, we obtain the kinetic equations for the model as

$$\nabla \cdot \mathbf{u} = 0, \tag{S19a}$$

$$\varrho \frac{D\mathbf{u}}{Dt} = -\nabla p + \nu \nabla^2 \mathbf{u} - \nabla \cdot \boldsymbol{\sigma}_K + \mathbf{b}, \tag{S19b}$$

$$\frac{\partial e}{\partial T} \frac{DT}{Dt} + \frac{\partial e}{\partial \rho} \frac{D\rho}{Dt} + \frac{\partial e}{\partial \phi} \frac{D\phi}{Dt} - \sum_j \frac{\partial e}{\partial \eta_j} \frac{D\eta_j}{Dt} = \nabla \cdot (\mathbf{k} \cdot \nabla T) + \boldsymbol{\sigma} : \nabla \mathbf{u} + q_v, \tag{S19c}$$

$$\frac{D\rho}{Dt} = \nabla \cdot \left[\mathbf{M} \cdot \nabla \frac{\delta \mathcal{F}}{\delta \rho} + \mathbf{M} \cdot \left(-\frac{\delta \mathcal{F}}{\delta \rho} \frac{\nabla T}{T} \right) \right], \tag{S19d}$$

$$\frac{D\phi}{Dt} = -L_\phi \frac{\delta \mathcal{F}}{\delta \phi}, \tag{S19e}$$

$$\frac{D\eta_j}{Dt} = -L_\eta \frac{\delta \mathcal{F}}{\delta \eta_j}, \tag{S19f}$$

with

$$\begin{aligned}
\frac{\delta \mathcal{F}}{\delta \rho} &= \frac{\partial f_{\text{loc}}}{\partial \rho} - T\kappa_\rho \nabla^2 \rho - T\kappa_\phi (\nabla^2 \rho - \nabla^2 \phi), \\
\frac{\delta \mathcal{F}}{\delta \phi} &= \frac{\partial f_{\text{loc}}}{\partial \phi} - T\kappa_\phi \nabla^2 \phi + T\kappa_\phi (\nabla^2 \rho - \nabla^2 \phi), \\
\frac{\delta \mathcal{F}}{\delta \eta_j} &= \frac{\partial f_{\text{loc}}}{\partial \eta_j} - T\kappa_\eta \nabla^2 \eta_j, \\
\sigma_K &= T\kappa_\rho \nabla \rho \otimes \nabla \rho + T\kappa_\phi \nabla \phi \otimes \nabla \phi + T\kappa_\phi (\nabla \rho - \nabla \phi) \otimes (\nabla \rho - \nabla \phi) + T\kappa_\eta \sum_j \nabla \eta_j \otimes \nabla \eta_j.
\end{aligned}$$

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