

Erratum: “Concurrent atomistic-continuum modeling of crystalline materials” [J. Appl. Phys. 126, 101101 (2019)]

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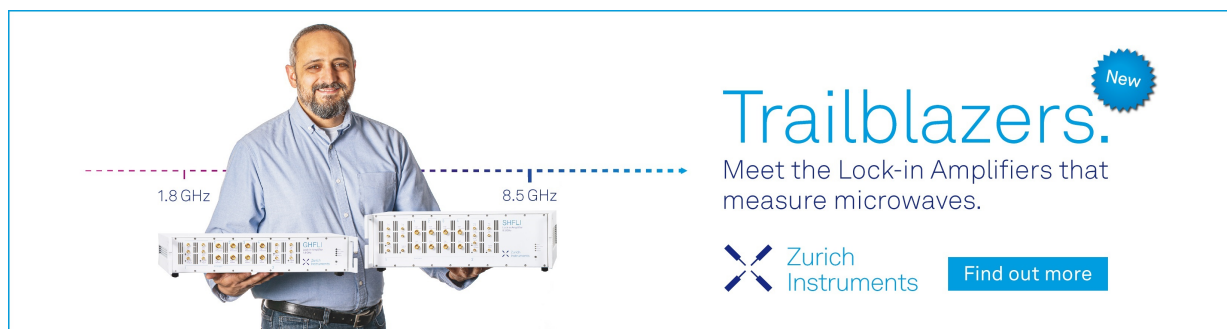
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There are typos in four of the equations in the original paper “Concurrent atomistic-continuum modeling of crystalline materials”¹ [J. Appl. Phys. **126**, 101101 (2019)]. These errors do not affect the final equations and the conclusions of the paper. We regret these errors and provide the correct equations as follows:

$$\delta_{V\alpha}(\mathbf{y} - \Delta\mathbf{r}_{k\xi}) \equiv \begin{cases} 1 & \text{if } \mathbf{y} - \Delta\mathbf{r}_{k\xi} \in V_\alpha \text{ or } \xi = \alpha, \\ 0 & \text{if } \mathbf{y} - \Delta\mathbf{r}_{k\xi} \notin V_\alpha \text{ or } \xi \neq \alpha. \end{cases} \quad (9)$$

In the original Eq. (9), we had the box function $\delta_{V\alpha}(\mathbf{y} - \Delta\mathbf{r}_{k\xi}) = 1$ for $\xi \neq \alpha$,

$$\begin{aligned} \frac{\partial(\rho_\alpha \mathbf{v}_\alpha)}{\partial t} &= \sum_{k=1}^{N_l} \sum_{\xi=1}^{N_a} m_\xi \tilde{\mathbf{v}}_{k\xi} \bar{\delta}_V(\mathbf{x} - \mathbf{r}_k) \bar{\delta}_{V\alpha}(\mathbf{y} - \Delta\mathbf{r}_{k\xi}) + \sum_{k=1}^{N_l} \sum_{\xi=1}^{N_a} m_\xi \mathbf{v}_{k\xi} \frac{\partial}{\partial t} \bar{\delta}_V(\mathbf{x} - \mathbf{r}_k) \bar{\delta}_{V\alpha}(\mathbf{y} - \Delta\mathbf{r}_{k\xi}) + \sum_{k=1}^{N_l} \sum_{\xi=1}^{N_a} m_\xi \mathbf{v}_{k\xi} \bar{\delta}_V(\mathbf{x} - \mathbf{r}_k) \frac{\partial}{\partial t} \bar{\delta}_{V\alpha}(\mathbf{y} - \Delta\mathbf{r}_{k\xi}) \\ &= \frac{1}{V} \oint_V (\mathbf{t}_\alpha - \rho_\alpha \mathbf{v}_\alpha \mathbf{v} \cdot \mathbf{n}) \cdot d\mathbf{S} + \frac{1}{V} \oint_{\partial V_\alpha} (\mathbf{t}_\alpha - \rho_\alpha \mathbf{v}_\alpha \Delta \mathbf{v}_\alpha \cdot \mathbf{n}) \cdot d\mathbf{S}_\alpha. \end{aligned} \quad (16)$$

In the original Eq. (16), “ $\frac{\partial}{\partial t}$ ” acted on both box functions in one of the terms in the right hand of the equation.

$$\int_{L_{kl}} \delta_A^n(\mathbf{x} - \boldsymbol{\varphi}) d\boldsymbol{\varphi} \equiv \frac{1}{A} \iint_{A^n} \int_{L_{kl}} \delta(\mathbf{x} + \mathbf{x}' - \boldsymbol{\varphi}) d\boldsymbol{\varphi} \cdot \mathbf{n} dS = \frac{1}{A} \begin{cases} 1 & \text{if } L_{kl} \text{ intersects } A^n \text{ and } \mathbf{n} \cdot \mathbf{L}_{kl} \geq 0, \\ -1 & \text{if } L_{kl} \text{ intersects } A^n \text{ and } \mathbf{n} \cdot \mathbf{L}_{kl} < 0, \\ 0 & \text{if } L_{kl} \text{ does not intersect } A^n. \end{cases} \quad (A3)$$

$$\bar{\delta}_A^n(\mathbf{x} - \mathbf{r}_k) \tilde{\mathbf{v}}_k \equiv \frac{1}{A \Delta t} \iint_{A^n} \int_0^{\Delta t} \delta(\mathbf{x} + \mathbf{x}' - \mathbf{r}_k) \tilde{\mathbf{v}}_k \cdot \mathbf{n} d\tau dS = \frac{1}{A \Delta t} \begin{cases} 1 & \text{if } \mathbf{r}_k \text{ intersects } A^n \text{ in } \Delta t \text{ and } \mathbf{n} \cdot \tilde{\mathbf{v}}_k \geq 0, \\ -1 & \text{if } \mathbf{r}_k \text{ intersects } A^n \text{ in } \Delta t \text{ and } \mathbf{n} \cdot \tilde{\mathbf{v}}_k < 0, \\ 0 & \text{if } \mathbf{r}_k \text{ does not intersect } A^n. \end{cases} \quad (A4)$$

In the original Eqs. (A2) and (A4), the centered dot “ $\cdot$ ” was misplaced.

REFERENCES

- ¹Y. Chen, S. Shabanov, and D. L. McDowell, [J. Appl. Phys.](#) **126**(10), 101101 (2019).