The Buckingham Catastrophe in multiscale modelling of fracture

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Abstract: Two original/modified Ball-Grimes models and one original/modified Lewis-Catlow models, are used in multiscale modelling of mixed mode fracture of Magnesia. The specimen is decomposed into a far field (modelled by linear elastic fracture mechanics), a near field (modelled by Atomistic Field Theory) and a crack-tip region (modelled by molecular dynamics). When two atoms get too close during the simulation of crack propagation, the attraction force artificially overcomes the repulsive barrier (Buckingham Catastrophe). The numerical results of three original models show significantly different phenomena. To demonstrate the sensitivity of interatomic potential and to prevent the catastrophe, three modified models are used. Numerical results of three modified models are compared and discussed.

Keywords: multiscale modelling; sensitivity of interatomic potential; magnesia; Coulomb-Buckingham potential; fracture mechanics; Buckingham Catastrophe.


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1 Introduction

Multiscale modelling provides the means to study local physical phenomena in a large structure with microstructural features. It is worthwhile to mention several different multiscale methods: variational multiscale methods (Hughes, 1995), homogenised Dirichlet projection method (Zohdi et al., 1996), domain decomposition methods (Xiao and Belytschko, 2004), Quasicontinuum (QC) method (Tadmor et al., 1996; Miller et al., 1998; Shenoy et al., 1999) and AFT (Chen and Lee, 2005; Chen, 2006; Chen, 2009).

In this work, a centre-cracked specimen made of magnesia is decomposed into three parts:

• far field, modelled by LEFM
• near field, modelled by AFT and analysed by a Generalised Atomistic Finite Element Method (GAFEM) (Lee et al., 2009)
• crack-tip region, modelled by MD.

The exact and analytical solution of the far field from LEFM is utilised to specify boundary conditions at the interface between the near field and the far field. Full-blown interatomic forces are employed between the near field and the crack-tip region.

Among all those multiscale approaches that use interatomic potentials, almost none studies the sensitivity of interatomic potentials and the Buckingham Catastrophe (Buckingham, 1938). Chen and Lee (2010) was the first to look into the Buckingham catastrophe and the sensitivity of interatomic potential during multiscale modelling of fracture. In this work, attention is focused on the investigation of how Buckingham catastrophe affects the modelling of fracture and the remedy to the catastrophe.

2 Theories for regions of different length scales

Let the centre-cracked specimen be decomposed into three parts. The far field is governed by the LEFM. In the crack-tip region, it is modelled by MD simulation. In between, named as the near field, it is modelled by AFT and simulated by GAFEM.

In LEFM, the exact and analytical Sneddon’s solution of displacement field for an infinite plate with a centre-crack, in 2D plane stress or plane strain case, can be expressed as (Sneddon and Lowengrub, 1969; Chen et al., 2006; cf. Figure 1):

\[
\begin{align*}
4\mu\varepsilon &= \frac{K_1}{\sqrt{\pi r_2}} \left[ (\kappa-1)r_2 \cos \frac{\theta + \theta_s}{2} - 2r_2^2 \sin \theta_s \sin \left( \theta_s - \frac{\theta + \theta_s}{2} \right) \right] \\
&+ \frac{K_2}{\sqrt{\pi r_2}} \left[ (\kappa+1)r_2 \sin \frac{\theta + \theta_s}{2} + 2r_2^2 \sin \theta_s \cos \left( \frac{\theta_s - \theta - \theta_s}{2} \right) \right] \\
&- 0.5r_2 \cos \theta_s (\sigma - \chi)(\kappa+1)
\end{align*}
\] (1)
The Buckingham Catastrophe in multiscale modelling of fracture

\[ 4\mu u = \frac{\kappa_1}{\sqrt{\pi \alpha}} \left[ (\kappa + 1)\alpha \sin \frac{\theta + \theta_1}{2} - 2r_1^2 \sin \theta_1 \cos \left( \frac{\theta - \theta_1}{2} \right) \right] \]

\[ + \frac{\kappa_2}{\sqrt{\pi \alpha r_2}} \left[ (1 - \kappa)\alpha \cos \frac{\theta + \theta_1}{2} + 2r_1^2 \sin \theta_1 \sin \left( \frac{\theta - \theta_1}{2} \right) \right] \]

\[ - 0.5r_1 \sin \theta_1 (\sigma - \chi)(\kappa - 3) \]  

(2)

where \( \mu \) is the shear modulus; \( u \) is the displacement; \( \kappa_1 = \sigma \sqrt{\pi \alpha} \); \( \kappa_2 = \tau \sqrt{\pi \alpha} \) and

\[ \kappa' = \frac{3 - 4\nu}{1 + \nu} \text{ for plane strain} \]

\[ \kappa' = \frac{3 - \nu}{1 + \nu} \text{ for plane stress} \]  

(3)

In this work, Sneddon’s solution is only used for the far field. In other words, the displacements along the interface between the near field and the far field are used as the boundary conditions imposed on the near field (cf. Figure 1 in Chen and Lee, 2010a; Chen et al., 2010).

**Figure 1** Geometry and loading condition of infinite centre-cracked specimen, where \( a \) is the half crack size

The near-field solution can be obtained through GAFEM based on the AFT, which can be reduced to MD simulation if the size of the element is reduced to the lattice constant. On the one hand, it is an atom-embedded continuum theory and therefore detailed atomic motion can be observed in the continuum region. On the other hand, it provides the accuracy close to MD simulation but in a much more computationally effective way. The balance law of linear momentum can be written as:
\[
\rho^\alpha \frac{\text{d}v^\alpha}{\text{d}t} = f^\alpha + \phi^\alpha + \nabla_{\alpha} \cdot \mathbf{r}_{\text{kinetic}}^\alpha + \nabla_{\rho'} \cdot \mathbf{r}_{\text{kinetic}}^\alpha
\]  

(4)

where the superscript \( \alpha \) refers to the \( \alpha \)th atom in the lattice cell; the terms on the RHD are, respectively, the inter atomic force density, the body force density, and the divergence of the kinetic part of homogeneous stress, \( \mathbf{r}_{\text{kinetic}}^\alpha \), and inhomogeneous stress, \( \mathbf{r}_{\text{kinetic}}^\alpha \), which are related to temperature (Lee et al., 2009). In the AFT, as in every continuum theory, temperature is an independent variable. This is different from MD simulation where temperature is a dependent variable, which can be computed through velocity field. In this work, only the interatomic force is considered. The weak form of a material system with \( N_g \) single crystals and \( N_a \) discrete atoms can be expressed as (Lee et al., 2009).

\[
\sum_{g=1}^{N_g} \int \Omega_g \sum_{\alpha=1}^{v(K)} \left\{ \rho^{\alpha,(K)} u^\alpha (K) - f^\alpha \right\} \cdot \delta u^\alpha (K) \text{d}\Omega_g + \sum_{i=1}^{N_a} \left\{ m^{\alpha(i)} u^i - F^i \right\} \cdot \delta u^i = 0. 
\]  

where \( v(K) \) is the number of atoms in a unit cell in \( K \)th crystal; \( \rho^{\alpha,(K)} \) is the mass density of the \( \alpha \)th atom in a unit cell of the \( K \)th crystal; \( u^\alpha (K) \) is the displacement of the \( \alpha \)th atom in a unit cell of the \( K \)th crystal; \( \Omega_g \) is the volume of \( K \)-th crystal; \( m^{\alpha(i)} \) is the mass of the \( i \)th atom in the discrete atomic region; \( u^i \) is the displacement of the \( i \)th atom in the discrete atomic region.

The crack-tip region is modelled by MD simulation:

\[
m \frac{d^2 r^i}{dt^2} = F^i = \sum_j F^{ij}.
\]  

(6)

\[
U^{ij} = \frac{Z^i Z^j}{r^{ij}} + A^i \left( \frac{r^{ij}}{\rho'} \right)^{6} - C^i \left( \rho'^{ij} \right)^{6} + D^{ij} \left( \rho'^{ij} \right)^{12}.
\]  

(7)

\[
F^{ij} = -\frac{\partial U^{ij}}{\partial r^{ij}} = \left\{ \frac{-Z^i Z^j}{(r^{ij})^6} + \frac{A^i}{B^i \rho'} \left( \frac{r^{ij}}{\rho'} \right)^5 + 6C^i \left( \rho'^{ij} \right)^2 - 12D^{ij} \left( \rho'^{ij} \right)^6 \right\} \left[ r^i - r^j \right].
\]

Equation (6) is Newton’s second law. The interatomic force is derived from the modified Coulomb-Buckingham potential, equations (7) and (8). Full-blown interatomic forces are employed in near field, in crack-tip region and between the two regions. Hence, there is no need to have an overlapping region or a special treatment for the interface.

Three different models, L-C model and two B-G models, of Coulomb-Buckingham potential for Magnesia (MgO) are utilised in this work (Henkelman et al., 2005). In L-C model and B-G I model, formal charges (\( \pm 2e \)) are assumed while in B-G II model partial charges (\( \pm 1.7e \)) are assumed. In these original models, \( D^i = 0 \). In Figure 2, it is seen that a potential barrier exists to prevent the collision of two oxygen atoms at a critical distance. This implies if the interatomic distance is less than the critical distance, the interatomic force changes from repulsive to attractive. The attractive force will make the interatomic distance even smaller and thus induces instability, which is unphysical and hence it is named Buckingham Catastrophe. It can also be seen that, from equation (7), when the interatomic distance is getting smaller, the \( -C^i (\rho'^{ij})^{-6} \) term dominates and approaches to negative infinity. It should be emphasised that the height of the barrier in B-G I model is almost four-fold of that in L-C model and B-G II model.
It explains why the B-G I model does not diverge easily. Here, we use the word ‘divergence’ to describe a state that the material system cannot find or maintain a new equilibrium so that the atoms are unable to withhold a certain order but move away from each other’s instead. The remedy term, $D^\alpha(r^\beta)^{-12}$, gives a barrier of infinite height and avoid the unphysical attractive force (Buckingham Catastrophe) between oxygen atoms at short range. Figure 3 shows the plot of interatomic potential vs. interatomic distance of three modified Coulomb-Buckingham potentials. It is seen that the difference between three original models are abated and the Buckingham Catastrophe has been avoided.

**Figure 2**  Interatomic potential of three models for O-O interaction of magnesia with Coulomb-Buckingham Potential

![Interatomic potential of three models for O-O interaction of magnesia with Coulomb-Buckingham Potential](source: Chen and Lee (2010b))

**Figure 3**  Interatomic potential of three models for O-O interaction of magnesia with Modified Coulomb-Buckingham Potentials

![Interatomic potential of three models for O-O interaction of magnesia with Modified Coulomb-Buckingham Potentials](source: Chen and Lee (2010b))

### 3 Simulation results and remedy

The material used in this work is magnesia. It has 8 atoms in a conventional unit cell. The entire solution domain, including the MD simulation region, has $141 \times 101 \times 3$ lattice points. The lattice constant is equal to 7.937 Bohr ($1$ Bohr = $5.291772108 \times 10^{-11}$ m). The relaxation time is equal to 4000 time steps.
Each time step is 40 atomic units. Each atomic unit in time is 0.02419 femto-second. Half of the crack size, $a$, is 10000 Bohr. The shear and tensile loading rate are both $=6.788 \times 10^{-8}$ Bohr/(Atomic unit in time) = 0.15m/s at the infinity of the specimen (cf. Figure 1).

Figure 4 displays the atomic positions in the neighbourhood of crack tip based on the three original models. After 4000 relaxation steps, the crystal has its own optimised lattice structure for each different model. The B-G II model and the L-C model diverge at the 17349th and 32734th steps, respectively. At 62500th step (last step in the simulation), B-G I model still does not diverge and the crack closes up in the wake of the advancing crack tip. It demonstrates that the MD simulation is very sensitive to interatomic potential; even for the same material, a slightly different potential leads to completely different results.

Figure 4 Results of original interatomic potentials (see online version for colours)

<table>
<thead>
<tr>
<th>L-C Model</th>
<th>B-G I Model</th>
<th>B-G II Model</th>
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<tbody>
<tr>
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<td><img src="image2.png" alt="Image" /></td>
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<tr>
<td><img src="image4.png" alt="Image" /></td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
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</tbody>
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Source: Chen and Lee (2010b)

Figure 5 displays the atomic positions in the neighbourhood of crack tip based on the three modified models. After relaxation, the modified B-G I, B-G II and L-C models diverge at 21394-th, 20568-th and 23968-th steps, respectively. One may see that, although the three modified models still yield slightly different results, the remedy term indeed eases the differences of the outcomes in the original models. This is due to the fact that, in the modified models, the unphysical phenomenon is prevented.
Similar to radiation damage, in fracture mechanics, atoms can get very close to each other. To prevent the disturbance of the energy level of the atomic shells, i.e., to activate the repulsion at very small distances, two approaches can be used. In a low-energy problem, a $r^{-12}$ term can simply be added. In a high-energy problem, Ziegler-Biersak-Litmark (ZBL) potential (Ziegler et al., 1985) is suggested and can be represented universally.

4 Conclusions

In this work, the specimen is idealised as an infinite plate with a centre crack and solved by different approaches in different regions of length scales. Between the classical fracture mechanics and the MD simulation, AFT bridges the gap. From the beginning to the end, one never loses the sight of atoms.

From Figure 2, the differences of three original models and Buckingham catastrophe can be witnessed. Those are the fundamental reason why the results of atomic motions are very much different for the same material in the same physical problem. Furthermore, in O-O interaction, when the interatomic distance is getting smaller and over the barrier, the dominating term will approach to negative infinity, meaning high attractive force, which induces the collision of two atoms with the same type of charges. This violates the physics. Figure 3 shows that adding the remedy term, $D^{r^{12}}$, corrects the wrong physics and still provides a reasonable interatomic potential.
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References

