Particle-base Simulations

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Introduction

Nomenclature

- \( d \) spacing between dense vertical cracks (DVCs)
- \( D \) Dundurs' parameter
- \( E_1 \), \( E_2 \) Young's Modulus of CMAS penetrated layer, unpenetrated material
- \( f \) volume fraction of porosity
- \( h \) CMAS-infiltration depth and depth of channel cracks
- \( H \) thickness of TBC layer (1 mm)
- \( k_1 \), \( k_2 \) thermal conductivity of CMAS penetrated layer, unpenetrated layer
- \( \ell \) length parameter proportional to \( h \)
- \( s \) spacing between channel cracks
- \( T \) penetrate temperature at CMAS penetration depth
- \( T_{\text{sub}} \) substrate temperature
- \( T_{\text{surf}} \) TBC surface temperature
- \( T_{\text{CMAS}} \) CMAS melting temperature (\( \sim 1220 \) °C)
- \( \Delta_1 T \) difference between the temperature drop at the surface and that at the substrate (defined in Fig. 9)
- \( \Delta_1 T_{\text{surf/sub}} \) allowable temperature difference across TBC to avert delamination.
- \( x \) distance into TBC layer from surface

Greek letters

- \( \alpha \) effective thermal expansion coefficient of coating
- \( \alpha_{\text{sub}} \) thermal expansion coefficient of substrate
- \( \Delta_1 \alpha \) difference in thermal expansion coefficient between substrate and coating
- \( \Gamma \) mode I toughness of CMAS penetrated DVCs within the TBC
- \( \Gamma_{\text{tbc}} \) mode I TBC toughness
- \( \nu_1 \), \( \nu_2 \) Poisson ratio of CMAS penetrated layer, unpenetrated layer
- \( \Pi \) piezo-spectroscopic coefficient
- \( \sigma_B \) in-plane biaxial stress
- \( \bar{\sigma}_B \) average in-plane tensile stress in CMAS layer

Terminology used in this article is summarized in Table 1 and defined in the text. Briefly, the plan view of a segment cut from a representative shroud (Fig. 1) indicates three distinct zones (denoted I, II and III). Spalls are present in zone III, as well as sub-surface delaminations (Fig. 2b). The delaminations within this zone occur at three levels identified in figure. 2. Crack morphologies

Sections normal to the surface were made using procedures described elsewhere [7]. Scanning electron and optical images (Figs. 2 and 3) summarize the various crack and delamination morphologies. Plan view optical images of planarized surfaces (Fig. 3a and b) provide complementary information.

Zones I and II exhibit a characteristic splat microstructure [8] with an array of through-thickness separations typical of "dense vertically cracked" (DVC) systems [9–11]. The DVCs have spacing, \( d \approx 0.2 \) mm (Figs. 2a and 3a). The TBC has its original (as-deposited) thickness and a thin deposit is superposed.

Table 1

<table>
<thead>
<tr>
<th>Feature</th>
<th>Terminology</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Affected area of shroud</td>
<td>Zone I Shallow CMAS penetration</td>
<td></td>
</tr>
<tr>
<td>Zone II</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Zone III Deep penetration of CMAS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Location of delamination</td>
<td>Level (i) Just above bond coat</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Level (ii) Just below CMAS</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Level (iii) Just beneath surface</td>
<td></td>
</tr>
<tr>
<td>Region of CMAS penetration</td>
<td>Sublayer A Upper region near-surface</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Sublayer B Lower region of CMAS</td>
<td></td>
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</tbody>
</table>

What? Why? How?

- Smoothed-particle hydrodynamics (SPH)
- Peridynamics
- Moving Least Squares (MLS)
- Discrete Element Method (DEM)

- Same equations apply regardless of cracks
- Cracks/damage “just happen” as a result of properties/loading

- All reduce to collection of interacting particles.
- “Meshless” = nodes, but no elements (i.e. no predefined connectivity)
- All involve intrinsic length scale (element size?)
- Involve calculation of derivatives (except for $v = 1/4$)
- **Most** utilize dynamic integration of equations of motion.
Examples: Silling’s peridynamics

- Inter/transgranular fracture
- Cracking (plates, membranes)
- Ballistics
- Fiber networks

Askari, et al. JOP, 2008
Silling and Bobaru, IJNLM, 2005
Outline

• Smoothed Particle Hydrodynamics (SPH)
• Peridynamics
• Peristatics* with GPUs (and weird particles)
• Concluding Remarks

*Caution: term has just been coined. Object or you are complicit. Thomas Moore, 1535 (ACE)
Smoothed Particle Hydrodynamics

- Navier-Stokes: equilibrium & linear viscous fluid:
  \[ \rho \frac{dv}{dt} = -\nabla p + \mu \nabla^2 v + f \]

- Want collection of particles to represent fluid:
  \[ a_i = \frac{dv_i}{dt} = \frac{F_i}{\rho_i}; \quad \ddot{r}_i = \frac{F_i(r, \dot{r})}{\rho_j(r)} \]
Smoothing Particle Hydrodynamics (SPH):

- The key to it all: (volume) smoothed (interpolated) quantities:
  \[ A(r) = \int_{\Omega(h)} A(r') W(r - r') \, dr \]

  \[ A(r) = \sum_j A_j V_j W(r - r_j) \quad V = \frac{m}{\rho} \quad A(r) = \sum_j A_j \frac{m_j}{\rho_j} W(r - r_j) \]

- For example, density:
  \[ \rho_i = \rho(r_i) = \sum_j \rho_j \left( \frac{m_j}{\rho_j} \right) W(r_i - r_j) = \sum_j m_j W(r_i - r_j) \]
Smoothed Particle Hydrodynamics: SPH

- Kernel (interpolation) function properties:

\[
\int_{\Omega(h)} W(r) dr = 1; \quad \lim_{h \to 0} W(r) = \delta(r); \quad W(r) \geq 0
\]

- \( h \) is critical, defines length-scale over which pressure/density are computed.

**Pressure**

\[
W(r, h) = \frac{315}{64\pi h^9} \left( h^2 - |r|^2 \right)^3; \quad 0 \leq |r| \leq h
\]

**Viscosity**

\[
W_\mu(r, h) = \frac{15}{2\pi h^3} \left( -\frac{|r|^3}{2h^3} + \frac{|r|^2}{h^2} + \frac{h}{2|r|} - 1 \right)
\]
Smoothed Particle Hydrodynamics: SPH

\[ \rho \frac{dv}{dt} = -\nabla p + \mu \nabla^2 v + f \]

• Need to compute gradients:

\[ \nabla A(r) = \sum_j A_j \left( \frac{m_j}{\rho_j} \right) \nabla W(r - r_j) \]

\[ f^p_i = -\nabla p(r_i) = -\sum_{j\neq i} p_j \left( \frac{m_j}{\rho_j} \right) \nabla W(r_i - r_j) \]

Note: \( p_j, \rho_j \) are functions of particle position!

• Gradients ‘pushed’ onto kernel functions, similar to FEA
Smoothed Particle Hydrodynamics: SPH

- More accurate way to compute derivatives:

\[ \rho \nabla A = \nabla (\rho A) - A \nabla \rho \rightarrow \nabla A = \frac{1}{\rho} (\nabla (\rho A) - A \nabla \rho) \]

- Force on particle due to pressure:

\[ f^p_i = -\rho_i \sum_{j \neq i} \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) m_j \nabla W (r_i - r_j) \]

Bulk modulus:

\[ p_i = \kappa (\rho_i - \rho_o) \]

- Force on particle due to viscosity:

\[ f^\mu_i = \mu \sum_j \left( \frac{m_i}{\rho_j} \right) (v_j - v_i) \nabla^2 W (r_i - r_j) = \mu \sum_j \left( \frac{m_i}{\rho_j} \right) (\dot{r}_j - \dot{r}_i) \nabla^2 W (r_i - r_j) \]
Smoothed Particle Hydrodynamics: SPH

\[ a_i = \frac{1}{\rho_i} \left( f_{-i}^p + f_{-i}^\mu \right) \]

\[ \rho_i = f(r_K) \quad \text{for all } K \text{ particles in } h \]

\[ f_{-i}^p = f(\rho_i) = f(r_K) \quad \text{for all } K \text{ particles in } h \]

\[ f_{-i}^\mu = f(\dot{r}_K, r_k) \quad \text{for all } K \text{ particles in } h \]

- Surface tension must be included.
- Must have enough particles.
- For any time step, ‘neighbors’ must be identified.
- Collision detection is needed for boundaries.
Smoothed Particle Elastodynamics: SPE

- Work through formalism for different constitutive law (different gradient terms)
- Time-stepping stepping slow: implicit algorithms slow.
- ‘Neighbors’ can be fixed for brittle materials (use cohesive laws to account for fracture)

Gray, Monaghan, Swift, Comp. Struc., 2001
Examples of SPH for elastodynamics:

Cleary and Das, IUTAM Symposium, 2008: elastic-plastic projectile

Cleary and Das, IUTAM Symposium, 2008: brittle compression
where $\alpha$ and $\nu$ with the Poisson ratio $\nu$ is the rotation tensor. The following equation of state is used:

$$\frac{\sigma_{ij}}{\rho} = \frac{K}{\mu} \delta_{ij} + \frac{\alpha}{\rho s} \bar{p} \delta_{ij}$$

where $\sigma_{ij}$ is the deviatoric stress, $\rho$ is the density, $K$ is the bulk modulus, $\mu$ is the shear modulus, $\alpha$ is a proportionality constant, and $\bar{p}$ is the mean pressure. The plasticity model used is a radial return plasticity model $S = s0 \bar{\epsilon}^p$. The trial stress $S$ is:

$$S_{ij} = (K/\mu) \delta_{ij} + \alpha \bar{p} \delta_{ij}$$

The plastic strain is incremented being the magnitude of the trial deviatoric stress $Tr = \sigma_{ij} - \frac{1}{3} Tr \delta_{ij}$ being the increment in equivalent plastic strain:

$$\epsilon^p_{eq} = \sqrt{\frac{2}{3} \sigma_{ij} \sigma^{ij}}$$

The final yield stress and $H$ is completed at 1150 ms and the blank takes on the shape of the die. Numerical simulation offers awesome capability to track properties and the history of each piece of metal is built into the part. Each SPH particle represents a specific volume of metal and the position of the air vents in turn depends on the gating system. The vents which enable the release of most of the entrapped air. The needs to have a good die design with accurate positioning of air vents and the gating systems and into the die. In order to obtain homogeneous cast components with minimal porosity and void formation one for manufacturing high volume and low cost metal compo-

For the case of lower $\mu$, the trial stress $S_{ij}$ is completed at 1150 ms and the blank takes on the shape of the die. Numerical simulation offers awesome capability to track properties and the history of each piece of metal is built into the part. Each SPH particle represents a specific volume of metal and the position of the air vents in turn depends on the gating system. The vents which enable the release of most of the entrapped air. The needs to have a good die design with accurate positioning of air vents and the gating systems and into the die. In order to obtain homogeneous cast components with minimal porosity and void formation one for manufacturing high volume and low cost metal compo-

To explore the effect of hardening modulus on material deformation, the previous simulation was repeated with hardening modulus, the surface of the blank at different stages of compaction is smooth. When a higher value of hardening modulus, the surface of the blank at different stages of compaction becomes rough. Again, we will discuss the possible advantages of SPH for forging in the context of defect prediction:

Severe surface oxidation (scale) can form if the metal is heated and face oxide has been effectively demonstrated in ingot casting. Again, we will discuss the possible advantages of SPH for forging in the context of defect prediction:

Our example also demonstrates prediction of one of the issues for the blank and the locations of high strain. The upper coloured by the plastic strain, and show the deformation pro-

Cleary, Prakash and Ha, J. Mat. Proc. Tech., 2006
Peridynamics (Silling)

- Two ‘flavors’:
  - **Bond-based**: simply pair interactions, $\nu = \frac{1}{4}$.
  - **State-based**: peridynamic stress and deformation tensors allow arbitrary constitutive models.

- Note based on PDEs (distinction with SPH) but reduces to PDEs in limit of refinement.

\[ f \] is somewhat ambiguous. Indeed, for a given function $u = u(x, t)$ the mathematical correct way to describe $f$ is using the Nemytskii operator $F : u \mapsto Fu$ with $(Fu)(x, \hat{x}, t) = f (\hat{x} - x, u(\hat{x}, t) - u(x, t))$. 

\[ 1 \] Note that the notation $f = f (\xi, \eta)$ is somewhat ambiguous. Indeed, for a given function $u = u(x, t)$ the mathematical correct way to describe $f$ is using the Nemytskii operator $F : u \mapsto Fu$ with $(Fu)(x, \hat{x}, t) = f (\hat{x} - x, u(\hat{x}, t) - u(x, t))$. 

Peridynamics

- The peridynamic equation of motion:

\[ \rho \ddot{u}(x, t) = \int_{\Omega(h)} f \left[ u(x', t) - u(x, t), x' - x \right] dV_{x'} \]

- The discretized form:

\[ \rho \ddot{u}_i = \sum_p f (u_p - u_i, x_p - x_i) V_p \]

- A sensible statement:

\[ \rho \ddot{u}_i = f_{ip} (dx^{ip}, du^{ip}) V_p \]
Peridynamics

- Bond stretch between particle “i” and particle “p“:

\[ s_{ip} = \frac{|dx^{ip} + du^{ip}| - |dx^{ip}|}{|dx^{ip}|} \]

- The constitutive law:

\[ |f_{ip}| = k \cdot s_{ip} \]

- Equivalent continuum properties:

\[ \kappa = \frac{\pi h^4 k}{18}; \quad v = \frac{1}{4} \quad G_c = \frac{9s_o^2 \kappa \delta}{5} \]
Peridynamics

- State-based model: compute peridynamic deformation and stress states
  - Map motion onto deformation gradient
  - Conventional stress-strain to get stress
  - Map stress onto bond forces

Silling, McMat07 (his website)
Examples: Silling’s peridynamics

*Inter/transgranular fracture*

Askari, et al. JOP, 2008

*Silling and Bobaru, IJNLM, 2005*

*Cracking (plates, membranes)*


*Ballistics*

*Fiber networks*
Peristatics* (with weird particles)
Rone Kwei Lim, William Pro, Professor Linda Petzold & Professor Marcel Utz (Southampton)

*(Most of) you are complicit.


Synthetic Al\textsubscript{2}O\textsubscript{3}/PMMA: Munch, et al., Science, 2008

Brick and mortar ‘particle’ modeling

- Small volumes of ceramics are strong.
- Small fractions of ductile phase limits compliance.
- Interlocking, ordered architecture transfers loads to bricks and diffuses damage.

Begley, et al., “Micromechanical models to guide the development of brick and mortar composites”, JMPS, 2012
Brick and mortar particle modeling

\[ \bar{E}_c = \frac{\bar{E}_c}{\bar{E}_b} = \frac{2(\sinh[\kappa_2]\kappa_1 - 2 \sinh[(-1 + \bar{s})\kappa_2] \sinh[\bar{s}\kappa_2] \kappa_2)}{2 \sinh[\kappa_2](1 + \kappa_1) + (\cosh[\kappa_2] - \cosh[(-1 + 2\bar{s})\kappa_2])\kappa_2} \]

- Subtle asymptotic limits: both small and large stiffnesses can be relevant

\[ \kappa_1 = \frac{E_m w}{E_b t_1} \]

\[ \kappa_2 = \sqrt{\frac{(1 - \nu_m)E_m w^2}{2E_b t_2 h}} \]

\[ \bar{E}_c = \frac{E_m w}{t} \left(1 + \frac{w}{12h}\right) \]

Begley, et al., “Micromechanical models to guide the development of brick and mortar composites”, JMPS, 2012
Brick and mortar particle modeling

• Only brick displacements & rotation matter.
• All energy at the system is in the interface.
• Cohesive law describes energy of the interface in terms of relative motion.
Brick and mortar particle modeling

![Graph showing interface energy and normal separation](image)
Brick and mortar particle modeling

**opening mode**

- Normal Traction, $T_n/\sigma_0$
- Normal Separation, $\Delta_n/(\delta_c+\delta_r)$

- Increasing sliding

**sliding mode**

- Tangential Traction, $T_t/\sigma_0$
- Tangential Separation, $\Delta_t/(\delta_c+\delta_r)$

- Increasing opening
Brick and mortar particle modeling

- Derivatives are expensive and localization is tough to capture. (---, ---)

- Connectivity is nearest neighbor and parallel function calls are cheap. (+++, ++++)

- Monte Carlo minimization (direct search)

- Calculate energy for new positions, accept lower energy states (and a small fraction of higher ones)
Brick and mortar particle modeling

Rone Kwei Lim, William Pro, Professor Linda Petzold
Brick and mortar particle modeling

Orientation of microstructure:

\[ \sigma_{Y^{90}}/\sigma_o = 2.75 \]

\[ E^{90}/h_k = 6.6 \]

\[ E^0/h_k = 1 \]

\[ \sigma_{Y^0}/\sigma_o = 1 \]

Timing Results For Various Code Improvements:

- CPU Code
- GPU Code
- GPU Code + Predictor
- GPU Code + Predictor + New Data Structure
Brick and mortar particle modeling

The computer version of Begley & Landes, 1972, ASTM STP 514

• Compute elastic energy (as a function of crack length, loading, geometry, etc.)
• Calculate the macroscopic energy release rate for the anisotropic elastic solid.
• Determine loads to initiate fracture, Infer initiation toughness.
• If toughness is actually a property, it should be independent of geometry and loading
Brick and mortar particle modeling

Vertical stress components, $\sigma_{22}/\sigma_0$

Distance from the crack tip, $a/W$
Brick and mortar particle modeling

Energy distribution
Brick and mortar particle modeling

Energy distribution: 90 degree case
“An Academic Life”
Screenplay by M.R. Begley & W. Pro

- Begley: “Plot the initiation toughness for all your specimens and loading conditions on a single plot.”
- (Pause for figure.)
- Begley: “Is this it?!?! I thought you ran like 100 cases. Plot them all.”
- William: “Why? They’re all pretty much identical.”
- (Pause for dumfounded stare.)
- William: “Oh. Yeah. We should do that.”
Brick and mortar particle modeling
Elastic brick and mortar particle modeling

Vertical Interface Toughness

0.06, 0.33
0.11, 0.11
0.08, 0.06

'onion peeling'

0.125, 0.33
0.25, 0.33

'delamination'

0.33, > 0.15
0.33, 0.11
0.33, < 0.1
0.33, < 0.06

'intact layers'

diffuse micro-cracking

'breaking'

Horizontal Interface Toughness

\[ \frac{\Gamma^H_i E_f}{8\sigma_f^2 h} \]
Concluding Remarks

Particle methods:

• Reduce complexity of meshing.
• Allow for discontinuities, geometry evolution.
• Can be adapted to a wide variety of constitutive models.
• Involve internal length scale: strongly impacts accuracy, speed.
• Calibration?!?!?