Surface treatment processing, model reduction and flowsheet implementation: high fidelity $\rightarrow$ reduced order (ML) $\rightarrow$ statistics

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Agenda

Lessons from Industrial Shot Peening (ISP) project, first principles to flowsheet.
Questions about reapplication to Cold Spray?
Thoughts on reapplication.

Model reduction approaches: high fidelity $\rightarrow$ reduced order (ML) $\rightarrow$ statistical models, e.g., in process flowsheets. Combine measures (e.g., particle size and shape distributions) with models (volume, area, number bases).

How can content of CSEE's Industrial Shot Peening (ISP) project be configured/extended to meet Sandia's surface engineering challenges, e.g., cold spray (CS)?

- Impingement of a particle-gas stream on a substrate;
- Interaction of particles and substrate (e.g., FEA);
- Model reduction strategy $\rightarrow$ process efficiency, product quality;
- Mass balance including a recycle stream;
- Recycle classification?

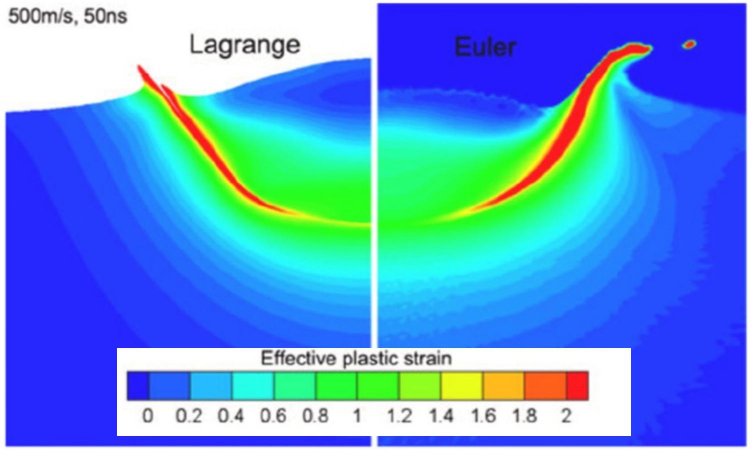
High fidelity models:

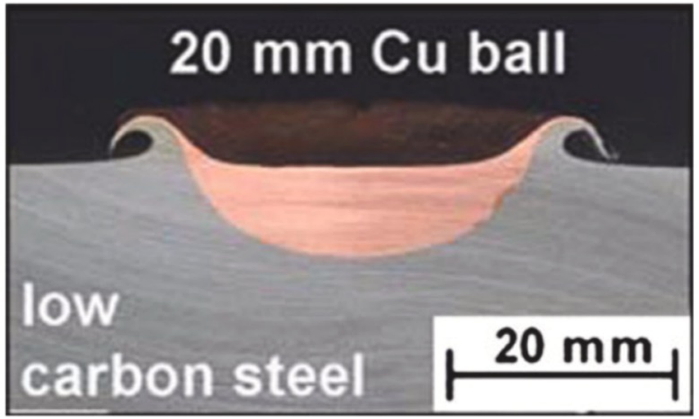
- ISP assumes elasto-plastic deformation of substrate and elastic media.
  - Models predict stress field in substrate and heterogeneity thereof.
    - Rep. vol. elements ($RVE_{substrate}$) >> iso-effect regions (iER_{media})
- CS requires plastic deformation of impinging particles; spreading $\Rightarrow$ expanded iER.
  - Model needs to predict build-up on substrate – iER interactions.
  - Residual stress state in substrate and/or built-up layer (RVE)?
  - Phase changes in deforming particles/layer?
  - What experimental methods exist to validate such a model?

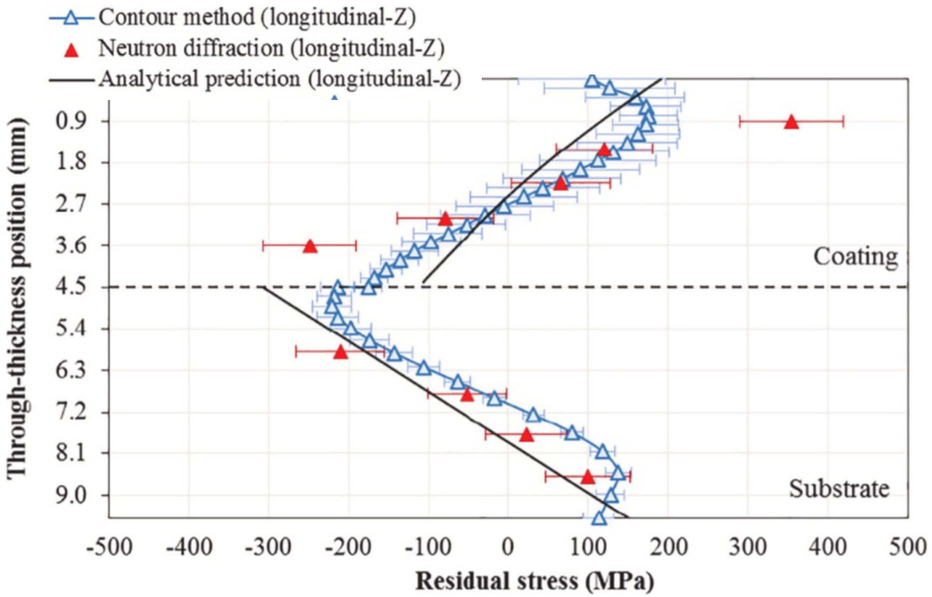
Reduced order:

- ML models of local heterogeneity
- Statistical prediction as a function of scale, stress, build-up:
  - RSD(scale of scrutiny)
- Mass balance including a recycle stream?
- Recycle classification?
- Dimensionality of desired model outputs?

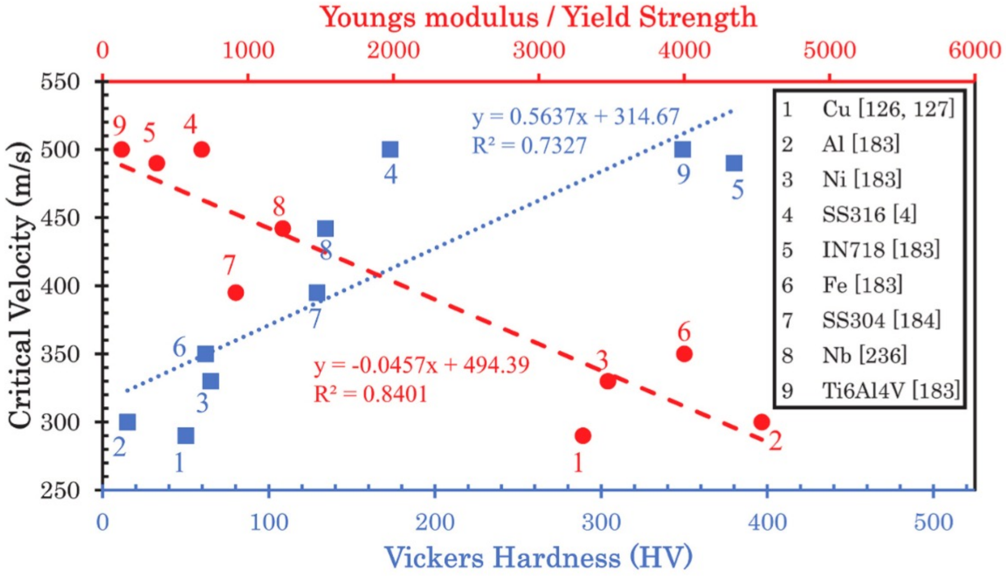
Preliminary Literature Review





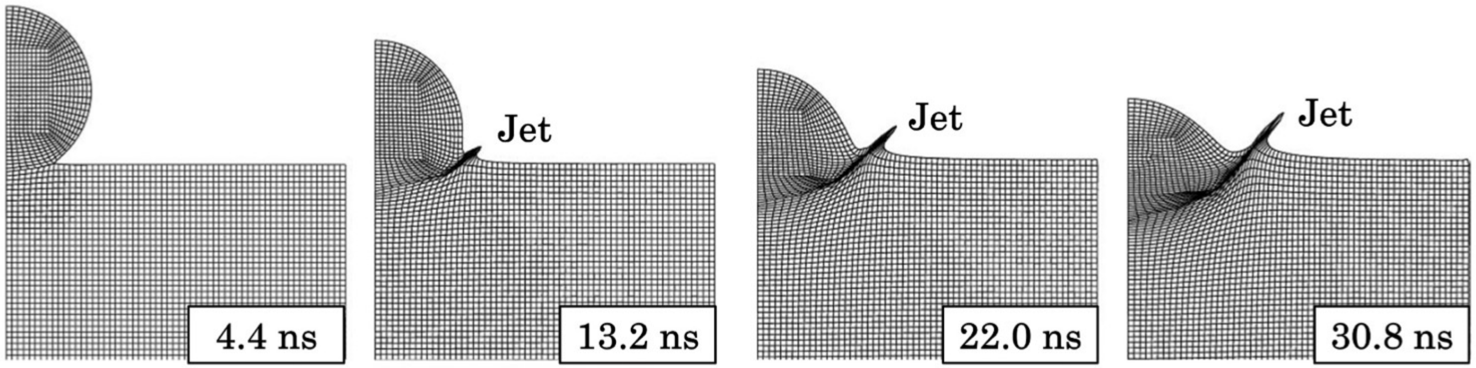


Historically, there is a significant amount of work on critical velocity and residual stresses in the substrate and deposited layer.



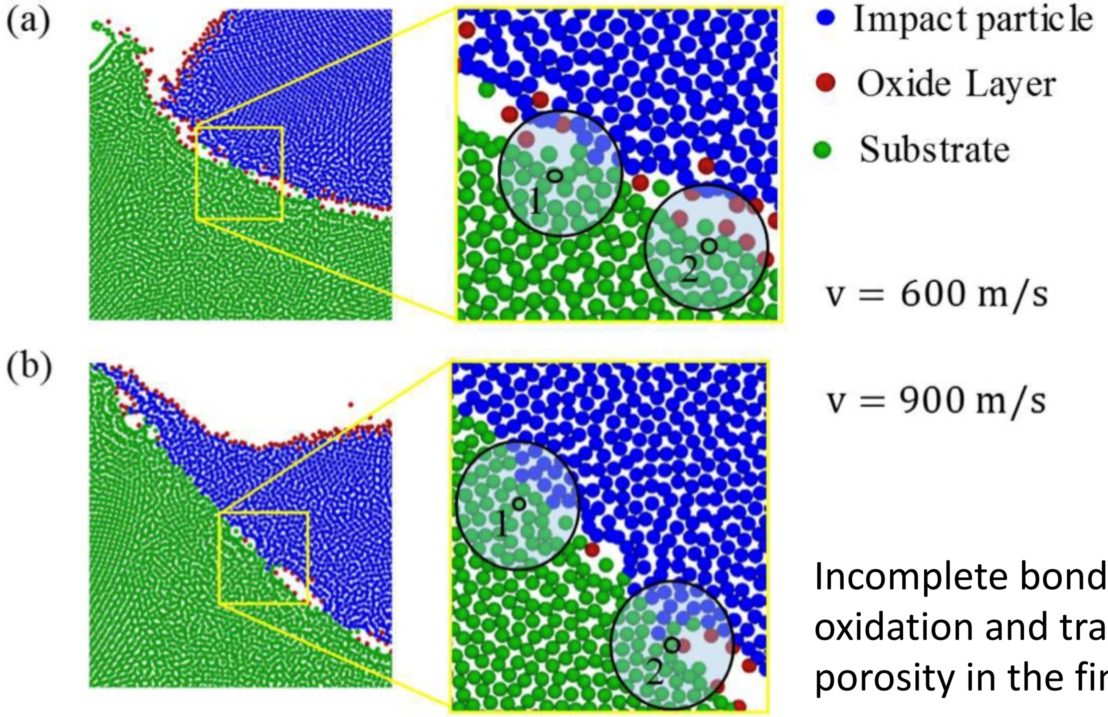
Fardan, A., Berndt, C. C., & Ahmed, R. (2021). Numerical modelling of particle impact and residual stresses in cold sprayed coatings: A review. *Surface and Coatings Technology*, *409*, 126835. https://doi.org/10.1016/J.SURFCOAT.2021.126835

Preliminary Literature Review

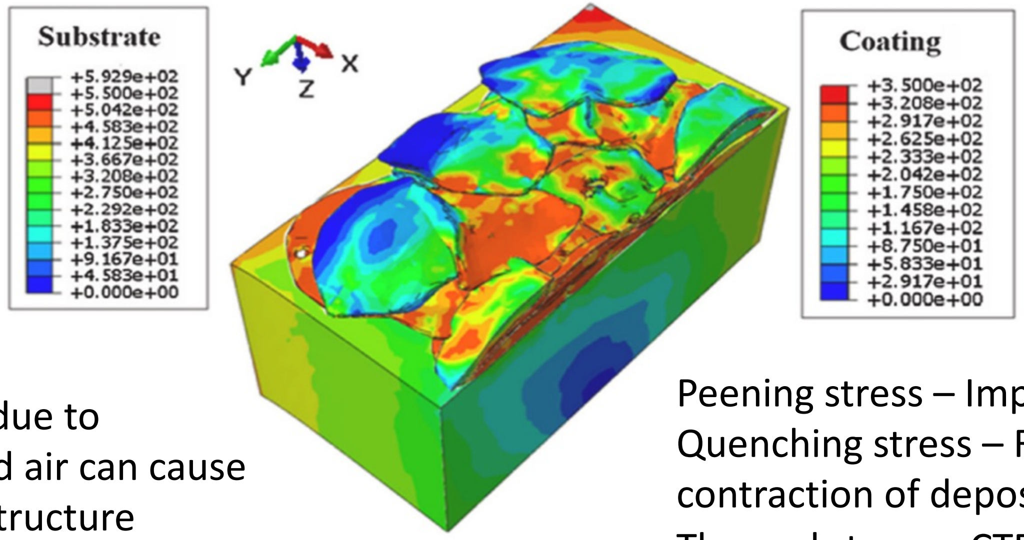


Thermal softening and local phase change cause jetting behavior at impact

Jetting and severe plasticity at interface make model building challenging and unpredictable. Interfacial interaction seems critical.



Significant residual stresses in both coating and substrate after processing



Incomplete bonding due to oxidation and trapped air can cause porosity in the final structure

Peening stress – Impact
Quenching stress – Restricted contraction of deposited layer
Thermal stress – CTE differential

Hemeda, A. A., Zhang, C., Hu, X. Y., Fukuda, D., Cote, D., Nault, I. M., Nardi, A., Champagne, V. K., Ma, Y., & Palko, J. W. (2021). Particle-based simulation of cold spray: Influence of oxide layer on impact process. *Additive Manufacturing*, *37*, 101517. https://doi.org/10.1016/J.ADDMA.2020.101517

Preliminary Literature Review – Simulation Overview

Several high-resolution modeling techniques have been used for cold-spray applications, with varying levels of success.

Table 1

Summary of the different modelling techniques for cold spray impact modelling.

Method	Advantages	Disadvantages	Computational efficiency	Computational accuracy
Lagrangian	+ Less computational time + Good particle/coating interface tracing	- Termination of the program due to high mesh distortion - Rebound of particles in multiple impacts	High computational effort and time to simulate extreme deformation	Low Due to highly deformed elements
Smoothed particle hydrodynamics (SPH)	+ Capable of modelling extreme deformation	- Less accuracy - Tensile instability - Fine mesh to obtain accurate results - Higher computational time and effort	High computational effort and time to obtain results comparable to other FE methods	Low Requires fine mesh to obtain results comparable to other FE methods
Eulerian	+ Capable of modelling extreme deformation + Deformation pattern is comparable to experimental observations	- Requires fine mesh which increases computational time. - Particle deformation and numerical results affected by mesh size - Particle coalescence - Inter-mixing of particle and substrate - Mass scaling cannot be used	Lower computational effort and time	Good
Coupled Eulerian Lagrangian	+ Capable of modelling extreme deformation + Allows to model interaction between particle and substrate	- Particle coalescence - Requires fine mesh which increases computational time.	Lower computational effort and time	Good
Molecular dynamics	+ Understanding the atomic level mechanism + Capability of modelling deformation of grain boundaries, phase transformations and dislocation movement	- Size effect (nano-level in MD vs micro-level in FEA) - Time limitation (simulate time period of 1–100 ns) - Describing equations of motion and interatomic interactions can be difficult	N/A Very high computational effort and time to simulate micron-sized particle impacts	N/A Difficult to compare MD with other FE method in terms of accuracy

The gold standard seems to be Eulerian methods.

Most legacy models are built in ABAQUS.

What we know:

Particle size and shape distributions are critical to CS, determining critical velocity, topography, and residual stress state.

Lagrangian FEA methods struggle with CS due to severe plasticity and jetting. SPH, Eulerian, MPM, MD can capture this better, but have trade-offs.

3 sources of stress that are critical to capture (Peening, Quenching, and Thermal).

Trapped air and incomplete bonding due to oxidation can cause porosity in the final structure.

What's missing?

All the highlighted models are high resolution and computationally intensive. Preliminary search did not find reduced-order numerical models of the cold-spray process.

Many legacy models consider only single impacts or limited coverage. We suspect that quasi-random impact locations will cause quantifiable variability in topography and residual stress state.

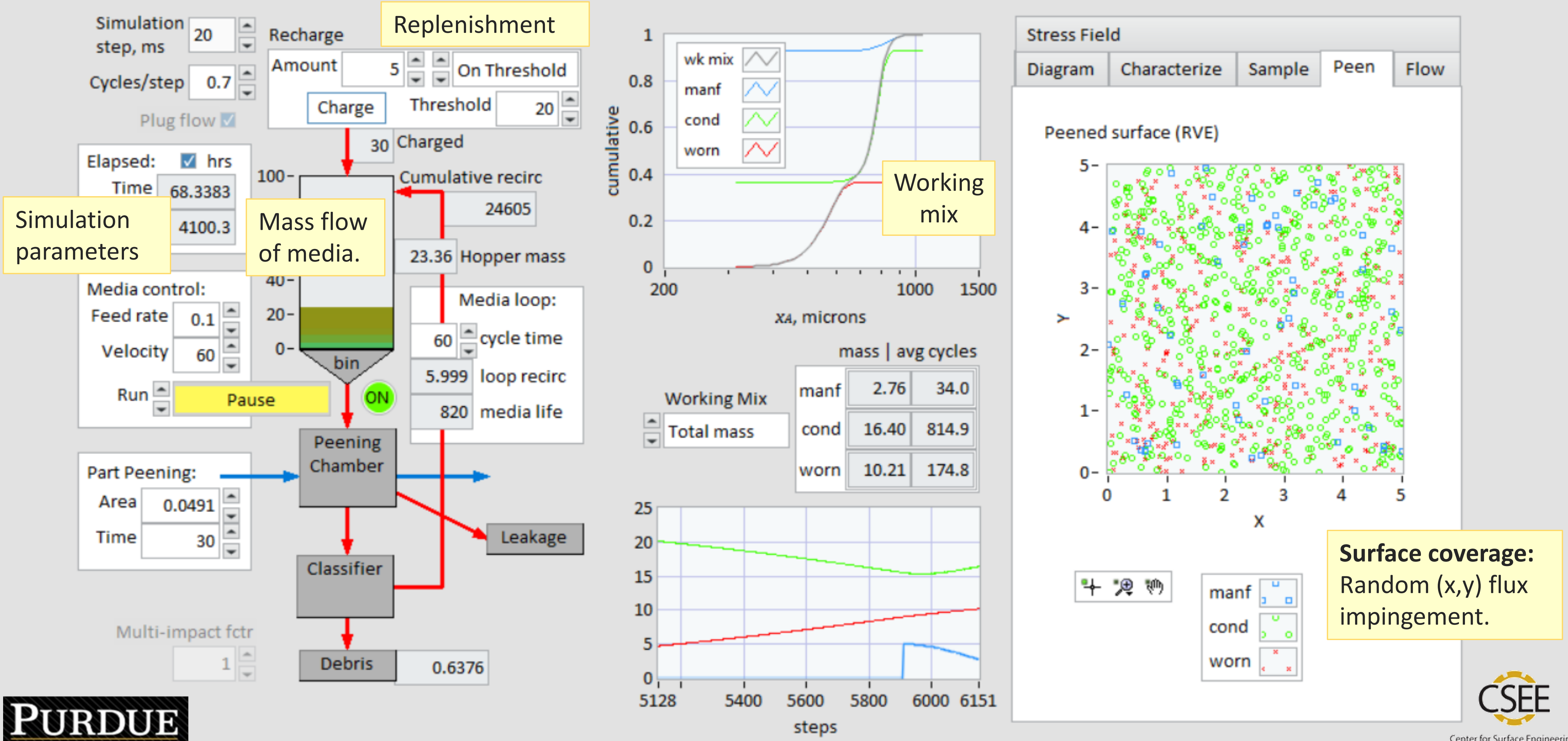
Integration into a flowsheet architecture. Tracking of virgin particle size and shape distributions and mixing with limited recycle loop of unplasticized media.

Distributions in impact velocity, particle size and shape, particle/substrate temperature along with stochastic process elements (impact arrangement and order) and their affect on uncertainty in outcome over a run of parts.

Process Flowsheet Modeling (ISP, Langdon Feltner)

Use reduced-order models to describe and predict dynamics in integrated systems.

- New applications, e.g., cold-spray, milling…



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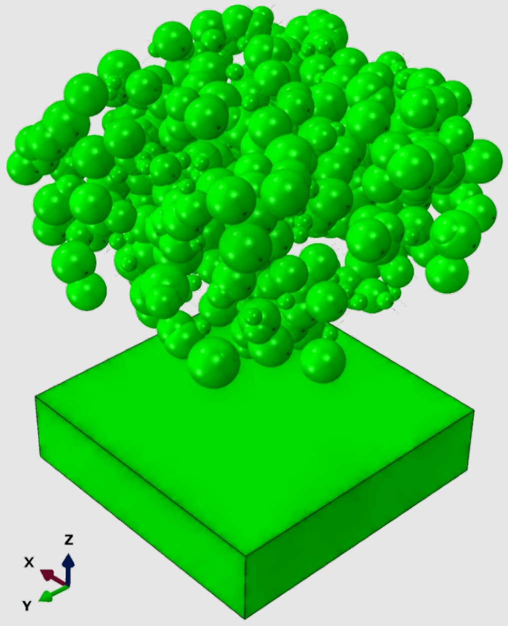
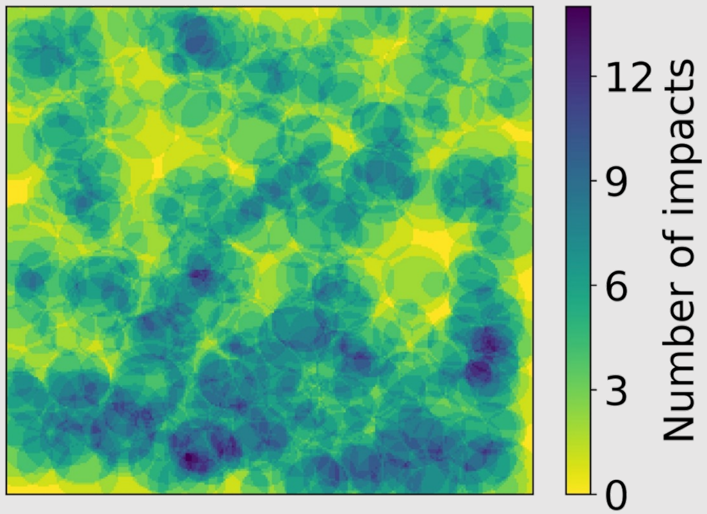
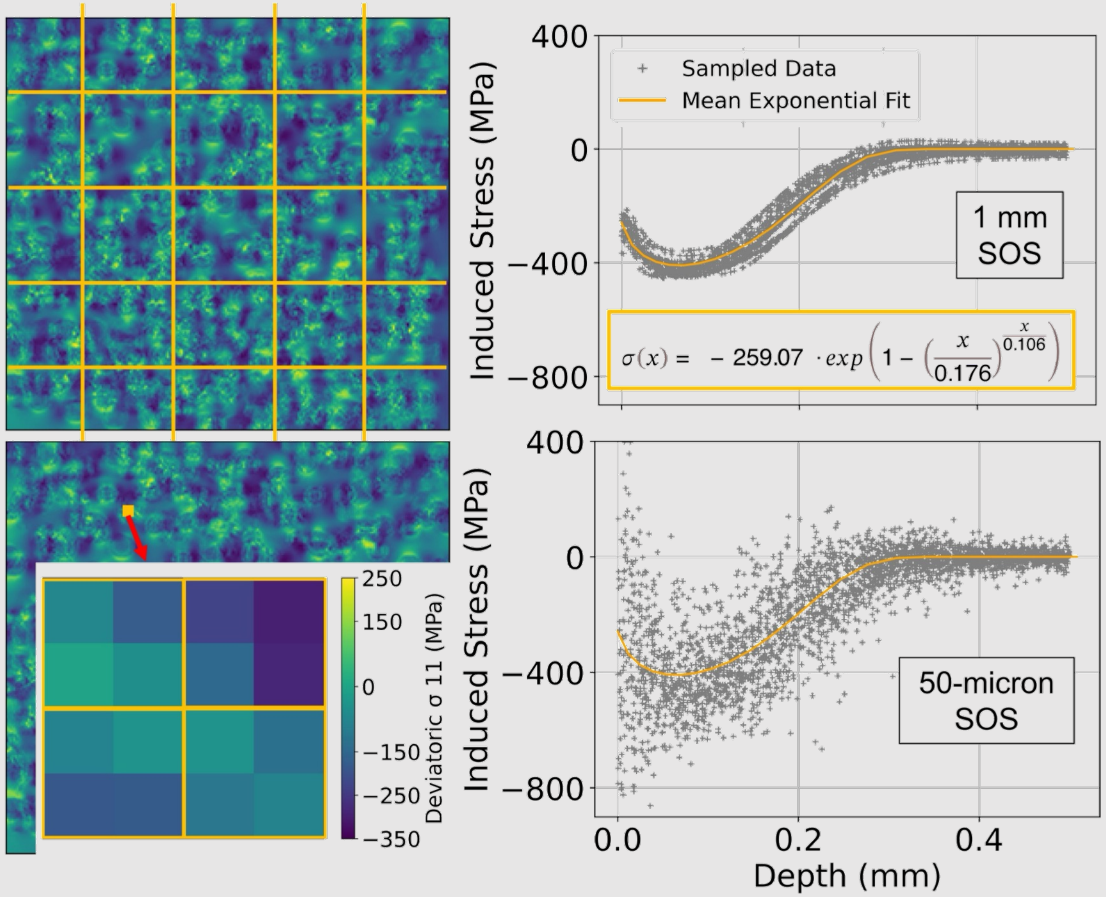
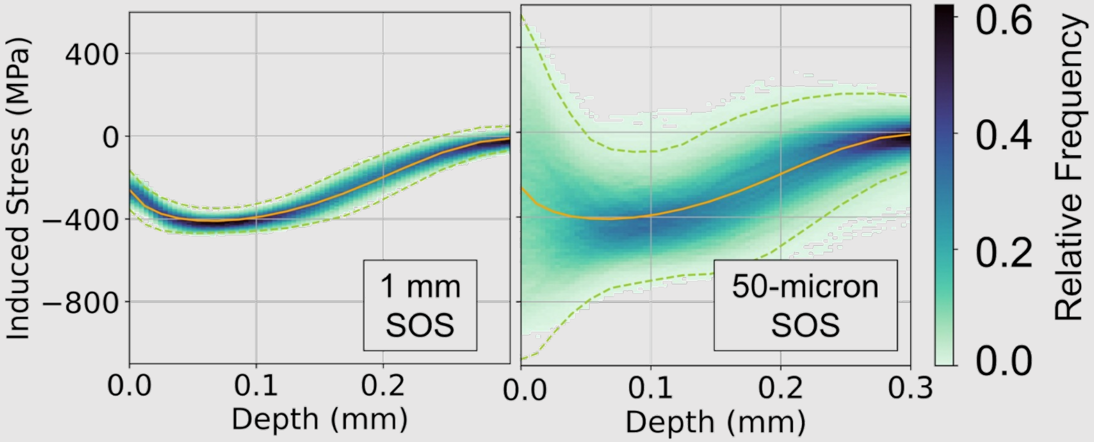
Stress Field Modeling in Context of Industrial Shot Peening (L. Feltner)









- Compressive stress fields imparted by shot peening have distributed surface and depth profiles relating to media characteristics and impact conditions.
- Variability depends on the local scale of scrutiny, i.e., in relation to a critical feature size of the part being treated.
- Model reduction (FEA → ML → statistics) enables use in flowsheets:
  - Actual media size and shape distributions,
  - Statistical variance of stress fields over a range of reference scales.