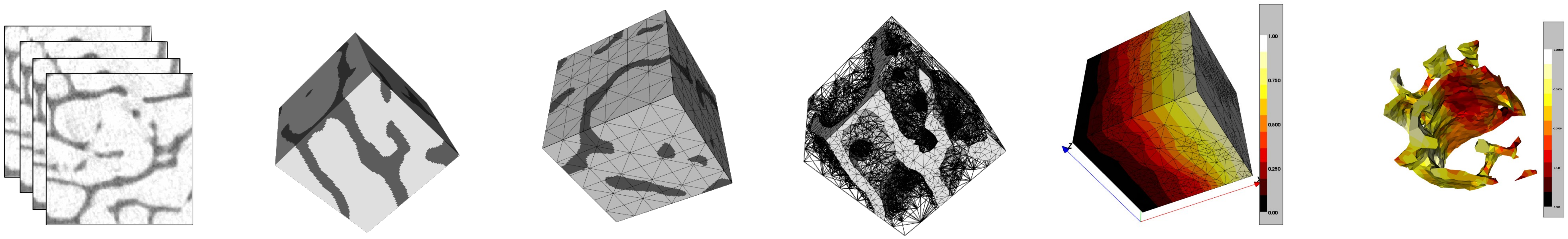
OOF: Open-source Finite Element Analysis for Materials

Andrew Reid (NIST), Stephen Langer (NIST), Shahriyar Keshavarz (Theiss Research)

National Institute of Standards and Technology
U.S. Department of Commerce

- The primary goal of the OOF project is to encapsulate sophisticated meshing and simulation tools for materials science audience
- The inputs are microstructural images, from experiment or simulation, and properties of the constituent phases
- It facilitates “structure-property exploration”, helping users examine how real microstructures behave under load
- Python and C++ object-oriented structure facilitates expansion



- **Workflow:** Begin with an image or set of images, use the segmentation tools to identify constituent phases. Then overlay a space-filling regular mesh, and use the mesh tools to make the mesh conformal with the constituent phases. Then, add the desired material properties, apply a load, and examine the result of the virtual experiment. Vary parameters and repeat as desired.
- The OOF platform provides tools for each of these steps – the user is assumed to be able to identify a good outcome, as these steps are hard to automate!

Math (Schematic, general case)

For some flux, σ (stress, heat flow, chemical flow) dependent on some field, ϕ (displacement, temperature, composition), solve for the divergence of the flux:

$$M \cdot \ddot{\phi} + C \cdot \dot{\phi} + \nabla \cdot \sigma + f = 0$$

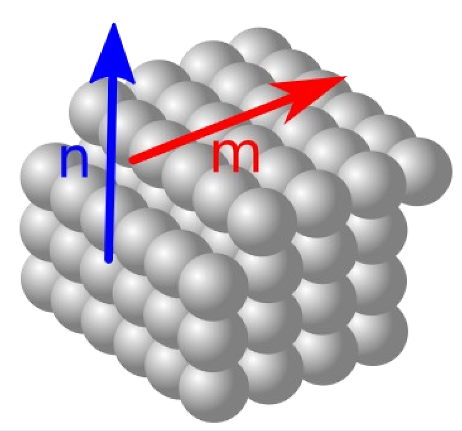
… with the constitutive rule governing how the flux depends on the fields, thus;

$$\sigma = \sum_i \gamma_i \nabla \dot{\phi} + \sum_i k_i \nabla \phi$$

We expect our users have lots of constitutive rules they want to try out.

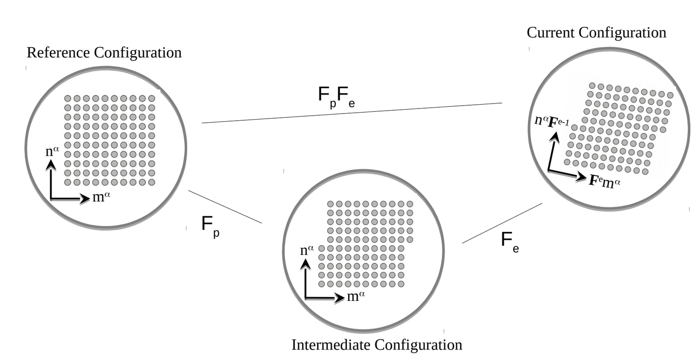
Development Focus: Crystal plasticity, an often-requested feature, which posed challenges!

- “Plasticity” is when materials take on a permanent deformation under load. “Crystal plasticity” is a model of this effect which is sensitive to the underlying crystallographic structure of the deforming material. It’s mostly relevant to metals.
- It’s much more than mechanical equilibrium! It includes many state variables, and incorporates history dependence.



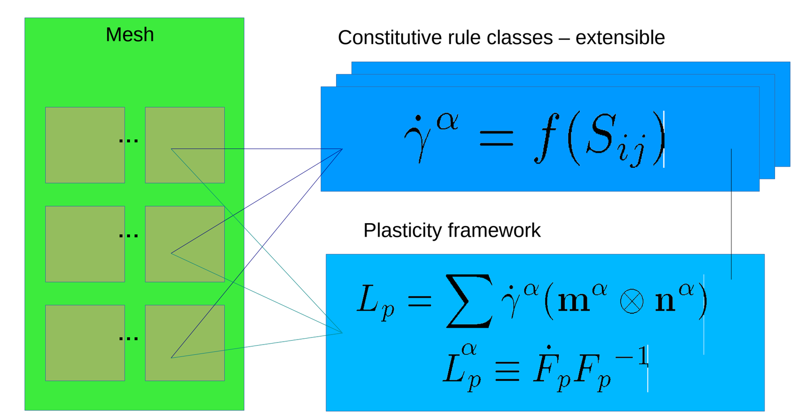
$$L_p = \sum_\alpha \dot{\gamma}^\alpha (\mathbf{m}^\alpha \otimes \mathbf{n}^\alpha)$$

Cartoon of the dislocation mechanism of crystal plasticity.



$$\dot{\gamma}^\alpha = f(S_{ij}) \quad L_p \equiv \dot{F}_p {F_p}^{-1}$$

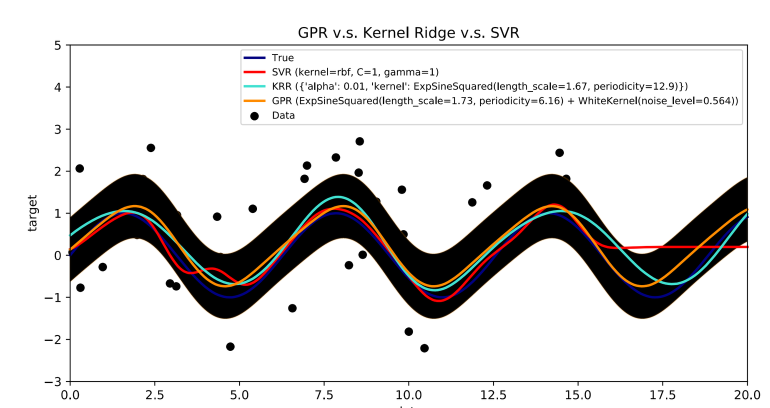
Multiple fields participate, in different spaces – mechanical equilibrium in “lab” space.



Crystal plasticity in OOF – object abstractions facilitate control over scopes, some architectural changes.

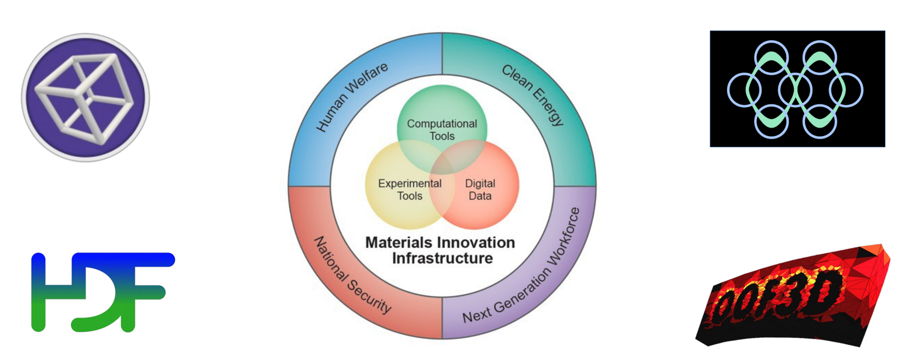
Roadmap items:

Accelerated evalution of constitutive rules by means of adaptively-sampled surrogate models.



The figure illustrates several 1D regression strategies, including Gaussian Process Regression, a common surrogate-model technique.
Image by Shiyu Ji, CC BY-SA 4.0

OOF should integrate with closed-loop materials modeling tool-chains to realize the benefits of integrated materials science and engineering.



Candidate tool-chains include Hyperthought and PRISMS, and data formats include Dream3D, as well as many other excellent projects working within the Materials Innovation Infrastructure effort of the Materials Genome Initiative.

There is an evident lack of **standard problems** in this field. NIST is well-positioned to use OOF to establish benchmarks for future plasticity codes