

## RESEARCH

# Materials Knowledge Systems in Python - A Data Science Framework for Accelerated Development of Hierarchical Materials

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## Abstract

To Do

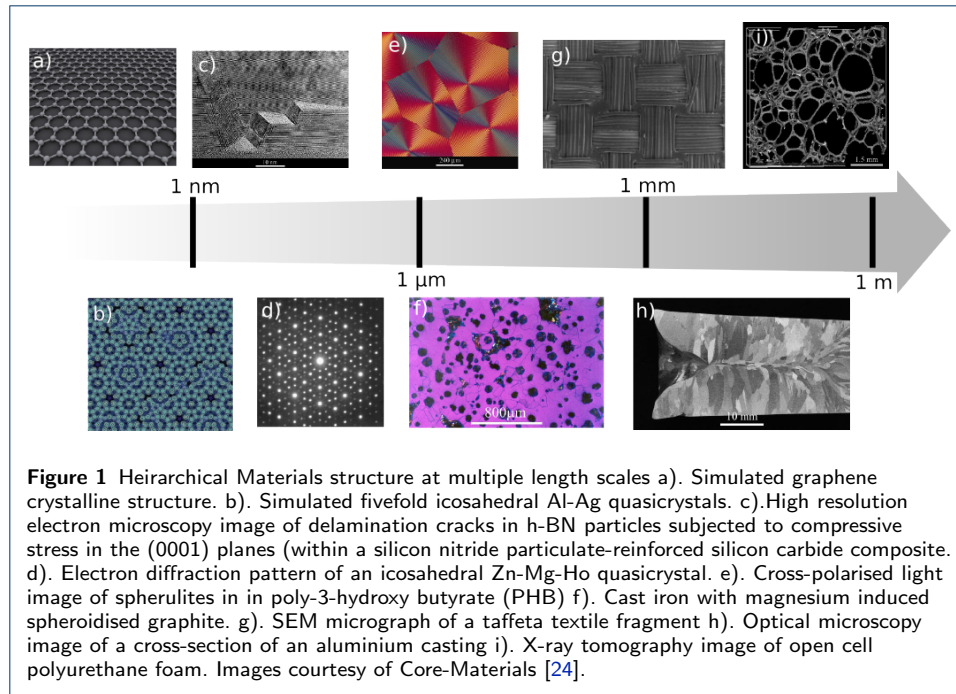
**Keywords:** TBD

## 1 Introduction

Current practices for developing tools and infrastructure used in multiscale materials design, development, and deployment are generally highly localized (sometimes even within a single organization) resulting in major inefficiencies (duplication of effort, lack of code review, not engaging the right talent for the right task, etc.). Although it is well known that the pace of discovery and innovation significantly increases with effective collaboration [1–4], scaling such efforts to large heterogeneous communities such as those engaged in materials innovation has been very difficult.

The advent of information technology has facilitated massive electronic collaborations (generally referred to as e-collaborations) that have led to significant advances in several domains including the discovery of the Higgs boson [5], the sequencing of the human genome [6], the Polymath project [7], the monitoring of species migration [8, 9] and numerous open source software projects. E-collaborations allow experts from complementary domains to create highly productive collaborations that transcend geographical, temporal, cultural, and organizational distances. E-collaborations require a supporting cyber-infrastructure that allows team members to generate, analyze, disseminate, access, and consume information at dramatically increased pace and/or quantity [10]. A key element of this emerging cyber-infrastructure is open source software as it eliminates collaboration hurdles due to software licenses and can help foster truly massive e-collaborations. In other words, even with collaborations involving proprietary data, open source cyber-infrastructure provides a common language that can facilitate e-collaborations with large numbers of team members (could even become a community effort).

Several recent national and international initiatives [11–13] have been launched with the premise that the adoption and utilization of modern data science and informatics toolsets offers a new opportunity to accelerate dramatically the design and deployment cycle of new advanced materials in commercial products. More specifically, it has been recognized that innovation cyber-ecosystems are needed to allow experts from the materials science and engineering, design and manufacturing, and data science domains to collaborate effectively. The challenge in integrating



these traditionally disconnected communities comes from the vast differences in how knowledge is captured, curated, and disseminated in these communities [14]. More specifically, knowledge systems in the materials field are rarely captured in a digital form. In order to create a modern materials innovation ecosystem, it is imperative that we design, develop, and launch novel collaboration platforms that allow automated distilling of materials knowledge from large amounts of heterogeneous data acquired through customized protocols that are necessarily diverse (elaborated next). It is also imperative that this curated materials knowledge is presented to the design and manufacturing experts in highly accessible (open) formats.

Customized materials design has great potential for impacting virtually all emerging technologies, with significant economic consequences [12, 13, 15–23]. However, materials design (including the design of a manufacturing process route) resulting in the combination of properties desired for a specific application is a highly challenging inverse problem due to the hierarchical nature of materials internal structure. Material properties are controlled by the hierarchical internal structure (over multiple length scales which spans from atomic to macroscopic) as well as coupled physical phenomena which can occur at different timescales at each of the hierarchical length scales. Characterization of the structure at each of these different length scales is often in the form of images which come from different experimental/computational techniques resulting in highly heterogeneous data. As a result, tailoring the material hierarchical structure to yield desired combinations of properties or performance characteristics is enormously difficult. Figure 1 provides a collection of materials images depicting material structures at different length scales, which are generally acquired using diverse protocols and are captured in equally diverse formats.

While the generation (from experiments and computer simulations) and dissemination of datasets consisting of heterogeneous images are necessary elements in

a modern materials innovation ecosystem, there is an equally critical need for customized analytics that take into account the stochastic nature of these data at multiple length scales in order to extract high value, transferable, knowledge. Data-driven Process-Structure-Property (PSP) linkages [25] provides a systemic, modular, and hierarchical framework for community engagement (i.e., several people making complementary or overlapping contributions to the overall curation of materials knowledge). Computationally cheap PSP linkages also communicate effectively the curated materials knowledge to design and manufacturing experts in highly accessible formats.

The Materials Knowledge Systems in Python project (PyMKS) is the first open source materials data analytics toolkit that can be used to create high value PSP linkages for hierarchical materials in large scale efforts driven and directed by an entire community of users. In this regard, it could be a foundational element of the cyber-infrastructure needed to realize a modern materials innovation ecosystem.

## 2 Current Materials Innovation Ecosystem

Open access materials databases and computational tools are critical components of the cyber-infrastructure needed to curate materials knowledge through effective e-collaborations [26]. Several materials science open source computational toolsets and databases have emerged in recent years to help realize the vision outlined in the Materials Genome Initiative (MGI) and the Integrated Computational Materials Engineering (ICME) paradigm [12, 13, 15–23]. Yet, the creation and adoption of a standard materials taxonomy and database schema has not been established due to the unwieldy size of material descriptors and heterogeneous data. Additionally, the coupled physical phenomena that govern material properties is too complex to model all aspects of a material simultaneously using a single computational tool. Consequently, current practices have resulted in the development of computation tools and databases with a narrow focus on specific length/structure scales, material classes, or properties.

NIST Data Gateway contains over 100 free and paid query-able web-based materials databases. These databases contain atomic structure, thermodynamics, kinetics, fundamental physical constants, x-ray spectroscopy, among other features [27]. NIST DSpace provides a curation of links to several materials community databases [28]. NIST Materials Data Curation Systems (MDCS) is a general online database that aims to facilitate the capturing, sharing, and transforming of materials data [29]. Open Quantum Materials Database (OQMD) is an open source data repository for phase diagrams and electronic ground states computed using density functional theory [30]. MatWeb is a database containing materials properties for over 100,000 materials [31]. Atomic FLOW of Materials Discovery (AFLOW) databases millions of materials and properties and hosts computational tools that can be used for atomic simulations [32]. The Materials Project (and the tool pyMatgen) [33, 34] provides open web-based access to computed information on known and predicted materials as well as analysis tools for electronic band structures. The Knowledgebase of Interatomic Models (OpenKIM) hosts open source tools for potentials for molecular simulation of materials [35]. PRedictive Integrated Structural Materials Science (PRISMS) hosts a suite of ICME tools and datastorage for

the metals community focused on microstructure evolution and mechanical properties [36].

SPPARKS Kinetic Monte Carlo Simulator (SPPARKS) is a parallel Monte Carlo code for on-lattice and off-lattice models [37]. MOOSE is a parallel computational framework for coupled systems of nonlinear equations [38]. Dream3D is a tool used for synthetic microstructures generation, image processing and mesh creation for finite element [39].

While there exists a sizable number of standard analytics tools [40–49], none of them are tailored to create PSP linkages from materials structure image data and their associated properties. PyMKS aims to seed and nurture an emergent user group in the materials data analytics for establishing homogenization and localization (PSP) linkages by leveraging open source signal processing and machine learning packages in Python. An overview of the PyMKS project accompanied with several examples is presented here. This paper is a call to others interested in participating in this open science activity.

### 3 Theoretical Foundations of Materials Knowledge Systems

Material properties are controlled by their internal structure and the diverse physical phenomena occurring at multiple time and length scales. Generalized composite theories [50, 51] have been developed for hierarchical materials exhibiting well separated length scales in their internal structure. Generally speaking, these theories either address homogenization (i.e., communication of effective properties associated with the structure at a given length scale to a higher length scale) or localization (i.e., spatiotemporal distribution of the imposed macroscale loading conditions to the lower length scale). Consequently, homogenization and localization are the essential building blocks in communicating the salient information in both directions between hierarchical length/structure scales in multiscale materials modeling. It is also pointed out that localization is significantly more difficult to establish, and implicitly provides a solution to homogenization.

The most sophisticated composite theory available today that explicitly accounts for the full details of the material internal structure (also simply referred as microstructure) comes from the use of perturbation theories and Green's functions [50, 52–63]. In this formalism, one usually arrives at a series expansion for both homogenization and localization, where the individual terms in the series involve convolution integrals with kernels based on Green's functions. This series expansion was refined and generalized by Adams and co-workers [62, 64, 65] through the introduction of the concept of a microstructure function, which conveniently separates each term in the series into a physics-dependent kernel (based on Green's functions) and a microstructure-dependent function (based on the formalism of  $n$ -point spatial correlations [56–61]).

Materials Knowledge Systems (MKS) [66–72] complement these sophisticated physics-based materials composite theories with a modern data science approach to create a versatile framework for extracting and curating multiscale PSP linkages. More specifically, MKS employs a discretized version of the composite theories mentioned earlier to gain major computational advantages. As a result, highly adaptable and templatable protocols have been created and used successfully to extract robust

and versatile homogenization and localization metamodels with impressive accuracy and broad applicability over large microstructure spaces.

The MKS framework is based on the notion of a microstructure function. The microstructure function provides a framework to represent quantities that describe material structure such as phase identifiers, lattice orientation, chemical composition, defect types and densities, among others (typically referred to as local states). The microstructure function,  $m_j(h; s)$ , represents a probability distribution for the given local state,  $h \in H$ , at each position,  $s \in S$ , in a given microstructure,  $j$  [73–76]. The introduction of the local state space  $H$  (i.e., the complete set of all potential local states) provides a consolidated variable space for combining the diverse attributes (often a combination of scalar and tensor quantities) needed to describe the local states in the material structure. The MKS framework requires a discretized description of  $m_j$ , which is denoted here as  $m_j[h; s]$ , where the  $[\cdot; \cdot]$  represent the discretized space (in contrast to  $(\cdot; \cdot)$ , which defines the continuous space). The “;” symbol divides indices in physical space to the right of “;” from indices in state space to the left of “;”. In most applications,  $S$  is simply tessellated into voxels on a regular (uniform) grid so that the position can be denoted by  $s \rightarrow i, j, k$  in three dimensions.

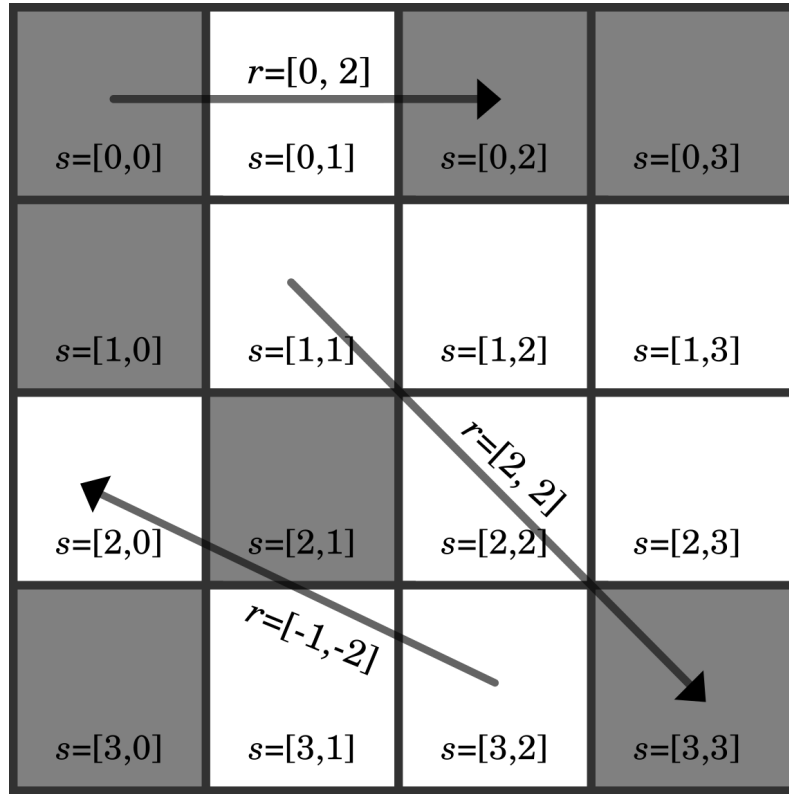
As noted earlier, the local state space in most advanced materials is likely to demand sophisticated representations. In prior work [68, 77, 78], it was found that spectral representations on functions on the local state space offered many advantages both in compact representation as well as in reducing the computational cost. In such cases,  $h$  indexes the spectral basis functions employed. The selection of these functions depends on the nature of local state descriptors. Examples include: (i) the primitive basis (or indicator functions) used to represent simple tessellation schemes [66, 67, 69–74, 79], (ii) generalized spherical harmonics used to represent functions over the orientation space [68, 77], and (iii) Legendre polynomials used to represent functions over the concentration space [78].

### 3.1 Homogenization

Comparing different microstructures is quite difficult even after expressing them in convenient discretized descriptions mainly due to the lack of a reference point or a natural origin for the index  $s$  in the tessellation of the microstructure volume. Yet the relative spatial distributions of the local states provide a valuable representation of the microstructure that can be used effectively to quantify the microstructure and compare it with other microstructures in robust and meaningful ways [72–74, 76, 79]. The lowest order of spatial correlations comes in the form of 2-point statistics and can be computed as a correlation of a microstructure function such that

$$f_j[h, h'; r] = \frac{1}{\Omega_j[r]} \sum_s m_j[h; s] m_j[h'; s + r] \quad (1)$$

where  $r$  is a discrete spatial vector within the voxelated domain specified by  $s$ ,  $f_j[h, h'; r]$  is one set of 2-point statistics for the local stats  $h$  and  $h'$  and  $\Omega_j[r]$  is a normalization factor that depends on  $r$  [79]. The subscript  $j$  refers to a sample microstructure used for analysis (i.e. each  $j$  could refer to a microstructure image). The physical interpretation of the 2-point statistics is explained in Fig. 2 with a



**Figure 2** The microstructure function (also referred to as the discretized microstructure) for a two phase composite material. Discrete vectors  $r$  describe the relative positions between different spatial locations.

highly simplified two-phase microstructure (the two phases are colored white and gray). If the primitive basis is used to discretize both the spatial domain and the local state space then  $f_j[h, h'; r]$  can be interpreted as the probability of finding local states  $h$  and  $h'$  at the tail and head of the vector  $r$ , respectively.

2-Point statistics provide a meaningful representation of the microstructure, but create an extremely large feature space that often contains redundant information. Dimensionality reduction can be used to create low dimensional microstructure descriptors from the sets of spatial correlations (based on different selections of  $h$  and  $h'$ ) with principal component analysis (PCA). The PCA dimensionality reduction can be mathematically expressed as

$$f_j[l] \approx \sum_{k \in K} \mu_j[k] \phi[k, l] + \overline{f[l]} \quad (2)$$

In Eq. 2,  $f_j[l]$  are the low rank approximations of 2-point statistics, where the  $f_j[h, h'; r]$  indices from Eq. 1 are represented as a vector with single index given by  $f_j[l]$  where  $l$  is a unique integer for every combination of  $h$ ,  $h'$  and  $r$ . The  $\mu_j[k]$  are low dimensional microstructure descriptors (the transformed 2-point statistics) or principal component scores (PC scores). The  $\phi[k, l]$  are the calibrated principle components (PCs) and the  $\overline{f[l]}$  are the mean values from the calibration ensemble

of  $f_j[l]$  for each  $l$ . The  $k \in K$  indices refer to the  $\mu_j[k]$  in decreasing order of significance and are independent of  $l$ ,  $l'$  and  $r$ . The main advantage of this approach is that the  $f_j[l]$  can be reconstructed to sufficient fidelity with only a small subset of  $\mu_j[k]$  [80].

After obtaining the needed dimensionality reduction in the representation of the material structure, machine learning models can be used to create homogenization PSP linkages of interest. As an example, a generic homogenization linkage can be expressed as

$$p_j^{\text{eff}} = \mathcal{F}(\mu_j[k]) \quad (3)$$

In Eq. 3,  $p_j^{\text{eff}}$  is the effective materials response (reflecting an effective property in structure-property linkages or an evolved low dimensional microstructure descriptor in process-structure linkages), and  $\mathcal{F}$  is a machine learning function that links  $\mu_j[k]$  to  $p_j^{\text{eff}}$ .

### 3.2 Localization

MKS Localization linkages are significantly more complex than the homogenization linkages. These are usually expressed in the same series forms that are derived in the general composite theories, while employing discretized kernels based on Green's functions [50, 52–63]. Mathematically, the MKS localization linkages are expressed as

$$p_j[s] = \sum_{h;r} \alpha[h;r] m_j[h;s-r] + \sum_{h,h';r,r'} \alpha[h,h';r,r'] m_j[h;s-r] m_j[h';s-r'] + \dots \quad (4)$$

In Eq. 4,  $p_j[s]$  is the spatially resolved (localized) response field (e.g. a response variable such as stress or strain rate in a structure-property linkage, or an evolved microstructure function in a process-structure linkage), and  $\alpha[h;r]$  are the Green's function based discretized influence kernels. These digital kernels are calibrated using regression methods [66–69, 77, 78].

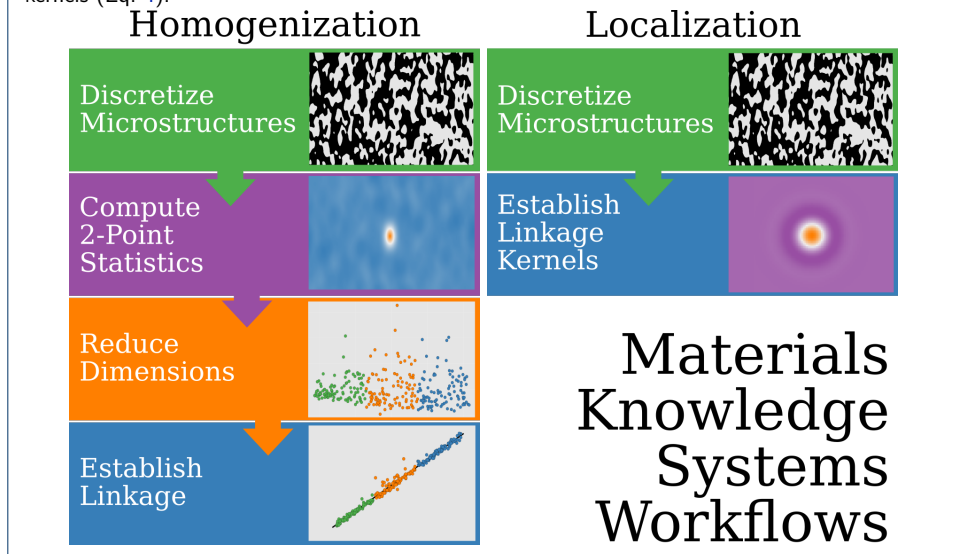
Fig. 3 provides a schematic overviews of the MKS homogenization and localization workflows. More detailed explanations on the MKS homogenization and localization linkages can be found in prior literature [66–74, 78, 79].

## 4 Materials Knowledge Systems in Python

PyMKS is an object-oriented numerical implementation to the MKS theory developed in the literature [67]. It provides a high-level, computational efficient framework to implement data pipelines for classification, cataloging and quantifying materials structures for PSP relationships. PyMKS is written in Python, a natural choice for scientific computing due to its ubiquitous use among the data science community as well as many other favorable attributes [81]. PyMKS is licensed under the permissive MIT license [82] which allows for unrestricted distribution in commercial and non-commercial systems.



**Figure 3** The MKS Homogenization workflow (left) consists of four steps. 1. Discretize the raw microstructure with the microstructure function. 2. Compute 2-point statistics using local states (Eq. 1). 3. Create low dimensional microstructure descriptors using dimensionality reduction techniques (Eq. 2). 4. Use machine learning model to establish a linkage with low dimensional microstructure descriptors. (Eq. 3). The MKS Localization workflow (right) consists of 2 steps. 1. Discretize the raw microstructure with the microstructure function. 2. Calibrated physics-based kernels (Eq. 4).



#### 4.1 Core Functionality

PyMKS consists of four main components including a set of tools to compute 2-point statistics, tools for both homogenization and localization linkages and tools for discretizing the microstructure. In addition, PyMKS has modules for generating data sets using conventional numerical simulations and a module for custom visualization of microstructures. PyMKS builds on Scikit-Learn’s pipelining methodology to create materials specific machine learning models. This is a high level system for combining multiple data and machine learning transformations into a single customizable pipeline with only minimal required code. This approach makes cross-validation and parameter searches simple to implement and avoids the complicated book keeping issues associated with training, testing and validating data pipelines in machine learning.

The starting point for an MKS homogenization analysis is to use 2-point statistics as outlined in Eq. 1 and provided in PyMKS by the `MKSStructureAnalysis` object, which calculates the objective low dimensional structure descriptors,  $\mu_j[k]$ . The default dimensionality reduction technique is PCA, but any model that uses the `transform_fit` or a “transformer” object can be substituted. After calculating the descriptors, the `MKSHomogenizationModel` is used to create linkages between the  $\mu_j[k]$  and the effective material response,  $p_j^{\text{eff}}$ , as indicated in Eq. 3. The default machine learning algorithm is a polynomial regression, but any estimator with the `fit` and `predict` methods can be substituted to create the linkages between  $\mu_j[k]$  and  $p_j^{\text{eff}}$ .

The `MKSLocalizationModel` object provides the MKS localization functionality. It calibrates the first order influence kernels  $\alpha[h;r]$  used to predict local materials responses,  $p_j[s]$ , as outlined in Eq. 4. The calibration of the influence kernels is



achieved using a variety of linear regression techniques described in numerous previous studies [66–68, 78]. The `MKSLocalizationModel` object uses `fit` and `predict` methods to follow the standard interface for a Scikit-learn estimator object.

To use either the homogenization or the localization models in PyMKS, the microstructure first needs to be represented by a microstructure function,  $m_j[h, s]$ . The `bases` module in PyMKS contains four transformer objects for generating the  $m_j[h, s]$  using a variety of discretization methods [66–72, 78]. These four objects can be thought of as materials specific extension to the feature extraction module in Scikit-Learn. A `PrimitiveBasis` object uses indicator (or hat) functions and is well suited for microstructures that have discrete local states (e.g., distinct thermodynamic phases). The `LegendreBasis` and `FourierBasis` objects create spectral representations of microstructure functions defined on nonperiodic and periodic continuous local state spaces, respectively. For example, functions over a range of chemical compositions can be described using `LegendreBasis`, while functions over orientations in two-dimensional space can be described using `FourierBasis`. Furthermore, `GSHBasis` creates compact spectral representations for functions over lattice orientation space (such as those needed to describe polycrystalline microstructures) [83–94].

PyMKS contains modest data generation tools (in the `datasets` module) that are used in both the PyMKS examples and the PyMKS test suite. The `MicrostructureGenerator` object creates stochastic microstructures using digital filters. This assists users in creating PyMKS workflows even when data is unavailable. PyMKS has objects for generating sample data from both a spinodal decomposition simulation (using the `CahnHilliardSimulation` object) and a linear elasticity simulation (using the `ElasticFESimulation` object). PyMKS comes with custom functions for visualizing microstructures in elegant ways (in the `tools` module). These are used extensively in the PyMKS example notebooks to minimize incidental code associated with visualization.

## 4.2 Underlying Technologies

PyMKS is built upon the highly optimized Python packages NumPy [95], SciPy [96], and Scikit-learn [42]. NumPy arrays are the primary data structure used throughout PyMKS and provide the basic vector and matrix manipulation operations. SciPy’s signal processing and numerical linear algebra functions are used to calibrate models and generate synthetic data. PyMKS is highly integrated with Scikit-learn and mimics its simple API in order to leverage from Scikit-learn’s data pipelining methodology for machine learning and data transformations. In addition, PyMKS uses the Pytest framework to automate execution of the test suite [97].

Optional packages that can be used with PyMKS include Simple Finite Elements in Python (SfePy) [98], the python wrapper for the FFTW library (pyFFTW) [99] and the plotting package Matplotlib [100]. SfePy is used to simulate linear elasticity to create sample response field data. PyFFTW is a highly optimized Fast Fourier Transform library that enhances the efficiency of PyMKS and enables parallel computations in PyMKS. Matplotlib is used to generate custom microstructure visualizations.

### 4.3 Development Practices

PyMKS leverages from existing tools, standards and web resources wherever possible. In particular the developers are an open community that use GitHub for issue tracking and release management (see <https://github.com/materialsinnovation/pymks>). Additionally a Google group is used as a public forum to discuss the project development, support and announcements (see [pymks-general@googlegroups.com](mailto:pymks-general@googlegroups.com)). The Travis CI continuous integration tool is used to automate running the test suite for branches of the code stored on GitHub. Code standards are maintained by following the Python PEP8 standards and by reviewing code using pull requests on GitHub. Detailed administrative guidelines are outlined in the `ADMINISTRATA.md` document and potential developers are encouraged to follow them.

## 5 Examples of Homogenization and Localization with PyMKS

Here a demonstration of the MKS homogenization and localization workflows as shown in Fig. 3 are presented using PyMKS. Additional workflow examples can be found on the PyMKS website [pymks.org](http://pymks.org).

### 5.1 Prediction of Effective Stiffness using Homogenization

#### 5.1.1 Calibration Data Generation

A set of periodic microstructures and their volume averaged elastic stress values  $\bar{\sigma}_{xx}$  can be generated by importing the `make_elastic_stress_random` function from `pymks.datasets`. This function has several arguments. `n_samples` is the number of samples that will be generated, `size` specifies the dimensions of the microstructures, `grain_size` controls the effective microstructure feature size, `elastic_modulus` and `poissons_ratio` are used to indicate the material property for each of the phases, `macro_strain` is the value of the applied uniaxial strain, and the `seed` can be used to change the the random number generator seed.

In this homogenization example, 200 samples from six different microstructures classes with dimensions 21 x 21 were created totaling 1,200 samples. Each of the six classes have different microstructure feature sizes. The `make_elastic_stress_random` function will return and the microstructures and their associated volume averaged stress values.

```
import numpy as np
from pymks.datasets import make_elastic_stress_random

sample_size = 200
grain_size = [(15, 2), (2, 15), (7, 7), (8, 3), (3, 9), (2, 2)]
n_samples = [sample_size] * 6
elastic_modulus = (310, 200)
poissons_ratio = (0.28, 0.3)
macro_strain = 0.001
size = (21, 21)

X, y = make_elastic_stress_random(
```

```
n_samples=n_samples, size=size, grain_size=grain_size,
elastic_modulus=elastic_modulus, poissons_ratio=poissons_ratio,
macro_strain=macro_strain, seed=0)
```

The microstructures can be visualized by importing `draw_microstructures`. Below is an instance from three of the classes.

```
from pymks.tools import draw_microstructures
```

```
X_examples = X[::sample_size]
draw_microstructures(X_examples[:3])
```



### 5.1.2 Calibration of Homogenization Model

In order to make an instance of the `MKSHomogenizationModel`, an instance of a basis class must first be created to specify the discretization methods for the microstructure microstructure function (see Fig. 3). For this particular example, there are only 2 discrete phases, therefore the `PrimitiveBasis` from `pymks.bases` will be used. The microstructure contain only two phases denoted by 0 and 1, therefore we have two local states and our domain is 0 to 1. An instance of the `PrimitiveBasis` with these parameters can be used to create an instance of the `MKSHomogenizationModel` as follows.

```
from pymks import MKSHomogenizationModel
from pymks.bases import PrimitiveBasis
```

```
p_basis = PrimitiveBasis(n_states=2, domain=[0, 1])
model = MKSHomogenizationModel(basis=p_basis, periodic_axes=[0, 1],
                               correlations=[(0, 0), (1, 1)])
```

The default pipeline used to create the homogenization linkage contains PCA and polynomial regression objects for Scikit-Learn. Cross validation is used on the testing data to find the optimal values (based on the R-squared values) within a defined subspace for our model parameters using `GridSearchCV` from `sklearn`. A dictionary `params_to_tune` defines the subspace with a range for the degrees of the polynomial and the number of principal components. For this example `n_components` will be varied between 2 to 11 and `degree` of the polynomial regression will be varied between 1 to 3.

```

from sklearn.grid_search import GridSearchCV

flat_shape = (X.shape[0],) + (X[0].size,)
params_to_tune = {'degree': np.arange(1,4),
                  'n_components': np.arange(2, 12)}
fit_params = {'size': X[0].shape}
gs = GridSearchCV(model, params_to_tune,
                  fit_params=fit_params).fit(X.reshape(flat_shape), y)

print('Order of Polynomial'), (gs.best_estimator_.degree)
print('Number of Components'), (gs.best_estimator_.n_components)
print('R-squared Value'), (gs.score(X.reshape(flat_shape), y))

```

```

Order of Polynomial 2
Number of Components 11
R-squared Value 0.999808062591

```

For the specified subspace it was found that a model with a 2nd order polynomial and 11 principal components had the highest R-squared value. The results over the whole subspace explored with GridSeachCV can be visualized using `draw_grid_scores`.

```

from pymks.tools import draw_gridscores

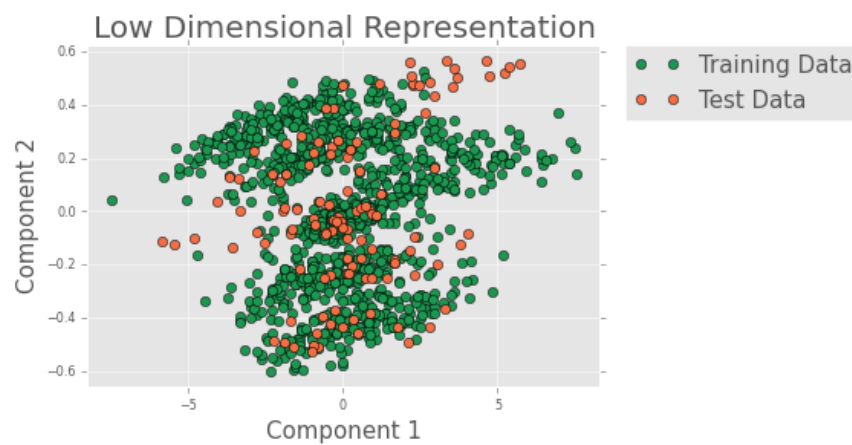
gs_deg_1 = [x for x in gs.grid_scores_
             if x.parameters['degree'] == 1][1:]
gs_deg_2 = [x for x in gs.grid_scores_
             if x.parameters['degree'] == 2][1:]
gs_deg_3 = [x for x in gs.grid_scores_
             if x.parameters['degree'] == 3][1:]

draw_gridscores([gs_deg_1, gs_deg_2, gs_deg_3], 'n_components',
                data_labels=['1st Order',
                             '2nd Order', '3rd Order'],
                param_label='Number of Components',
                score_label='R-Squared')

```



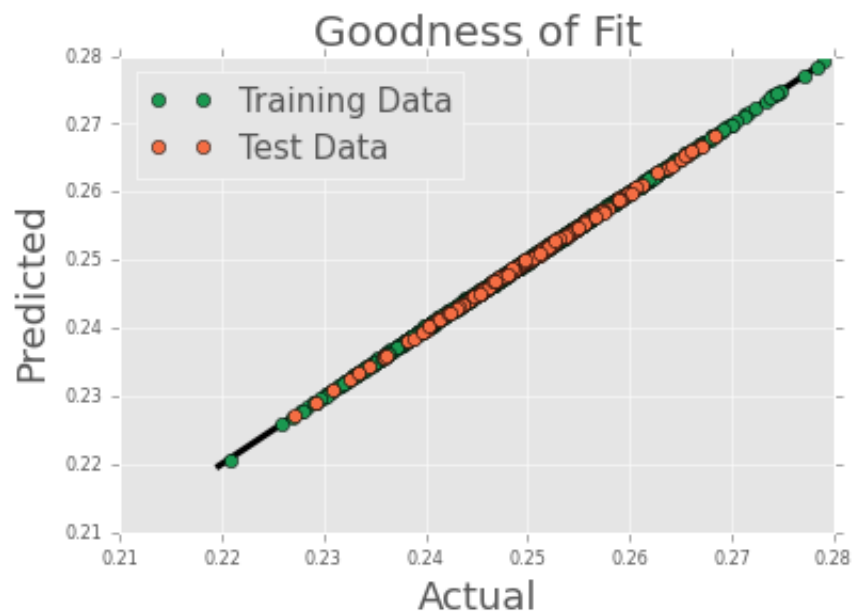
```
['Training Data', 'Test Data'])
```



The calibration and validation data are samples from the same distributions as expected. A goodness-of-fit plot provides a visualization of the models performance, and can be created by importing `draw_goodness_of_fit` from `pymks.tools`.

```
from pymks.tools import draw_goodness_of_fit
```

```
fit_data = np.array([y, model.predict(X)])
pred_data = np.array([y_new, y_predict])
draw_goodness_of_fit(fit_data, pred_data,
                    ['Training Data', 'Test Data'])
```



## 5.2 Prediction of Local Strain Field with Localization

### 5.2.1 Calibration Data Generation

In this example the `MKSLocalizationModel` used to predict the local strain field for a three phase microstructure with elastic moduli values of 80, 100 and 120; Poisson's ratio values all equal to 0.3 and a macroscopic imposed strain equal to 0.02.

The mode is calibrated using delta microstructures for the calibrated using delta microstructures (analogous to using a unit impulse response to find the kernel of a system in signal processing). The the material parameters specified above are used in a finite element simulation and must be passed into the `make_elasticFEstrain_delta` function from `pymks.datasets`. The number of Poisson's ratio values and elastic moduli values indicates the number of phases.

```
from pymks.tools import draw_microstructures
from pymks.datasets import make_delta_microstructures
import numpy as np

n = 21
n_phases = 3

from pymks.datasets import make_elastic_FE_strain_delta
from pymks.tools import draw_microstructure_strain

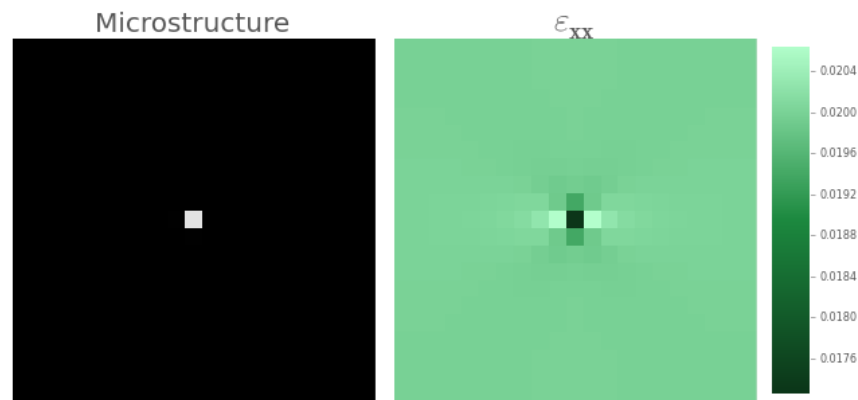
elastic_modulus = (80, 100, 120)
poissons_ratio = (0.3, 0.3, 0.3)
macro_strain = 0.02
size = (n, n)

X_delta, strains_delta = make_elastic_FE_strain_delta(
    elastic_modulus=elastic_modulus,
    poissons_ratio=poissons_ratio,
    size=size, macro_strain=macro_strain)
```

Delta microstructures are composed of only two phases with the center of the microstructure being a different phase from the rest. All permutations of thes delta microstructures and their associated strain fields  $\varepsilon_{xx}$  are needed to create calibrate the model. A delta microstructure and it's strain field can be visualized using `draw_microstructure_strain` for `pymks.tools`.

```
draw_microstructure_strain(X_delta[0], strains_delta[0])
```





### 5.2.2 Calibration of the Localization Model

In order to make an instance of the `MKSHomogenizationModel`, an instance of a basis class must first be created to specify the discretization methods for the microstructure microstructure function (see Fig. 3). For this particular example, there are only 2 discrete phases, therefore the `PrimitiveBasis` from `pymks.bases` will be used. The microstructure contain only two phases denoted by 0 and 1, therefore we have two local states and our domain is 0 to 1. An instance of the `PrimitiveBasis` with these parameters can be used to create an instance of the `MKSHomogenizationModel` as follows.

Similar to the `MKSHomogenizationModel`, an instance of a basis class to specify the discretization methods for the microstructure microstructure function (see Fig. 3). before an instance of the `MKSLocalizationModel` is created. An instance of `PrimitiveBasis` with `n_states` equal to 3, is used because the material system as 3 distinct phases.

```
from pymks import MKSLocalizationModel
from pymks import PrimitiveBasis

p_basis = PrimitiveBasis(n_states=3, domain=[0, 2])
model = MKSLocalizationModel(basis=p_basis)
```

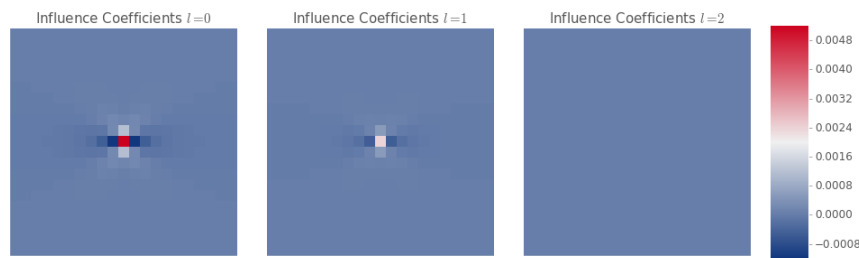
With the delta microstructures and their strain fields, the the influence kernels can be calibrated using the `fit` method.

```
model.fit(X_delta, strains_delta)
```

A visualization of the influence kernels can be generated using the `draw_coeff` function from `pymks.tools`.

```
from pymks.tools import draw_coeff

draw_coeff(model.coef_)
```

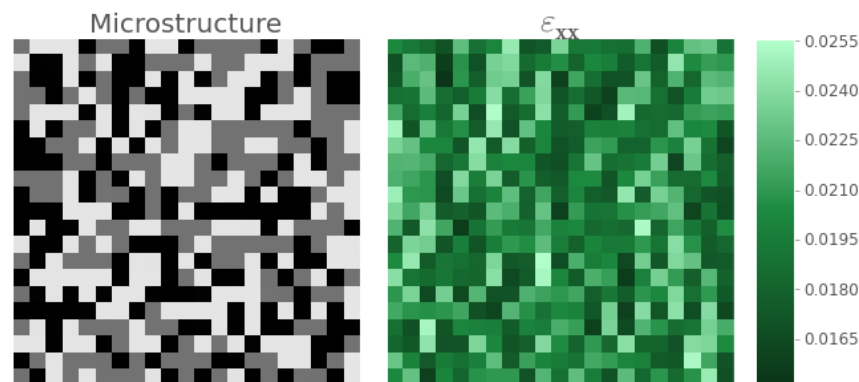


### 5.2.3 Prediction of the Strain Field for a Random Microstructure

A predicted strain field from the localization model can be compared the strain field using a finite element simulation for the same random microstructure for model validation. The `make_elasticFEstrain_random` function from `pymks.datasets` generates a random microstructure and its strain field results from finite element analysis.

```
from pymks.datasets import make_elastic_FE_strain_random
```

```
np.random.seed(101)
X, strain = make_elastic_FE_strain_random(
    n_samples=1, elastic_modulus=elastic_modulus,
    poissons_ratio=poissons_ratio, size=size,
    macro_strain=macro_strain)
draw_microstructure_strain(X[0], strain[0])
```



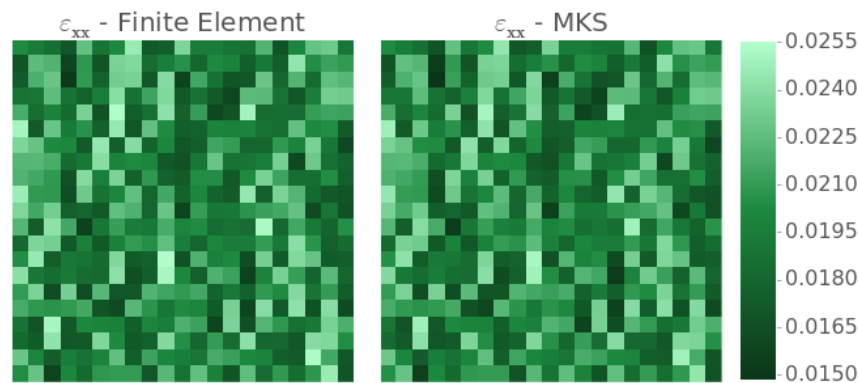
Localization model predicts the strain field by passing the microstructure to the `predict` method.

```
strain_pred = model.predict(X)
```

A visualization of the two strain fields from both the localization model and finite element analysis can be created using `draw_strains_compare` from `pymks.tools`.

```
from pymks.tools import draw_strains_compare

draw_strains_compare(strain[0], strain_pred[0])
```



## 6 Conclusion

PyMKS is an open source project with a permissive license that provides simple high level APIs to the MKS framework by implementing pipelines from Scikit-learn with customized objects for data from hierarchical materials. PyMKS developers is eager to collaborate with others to grow an emergent data science community for establishing homogenization and localization Process-Structure-Property linkages for hierarchical materials.

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