The hierarchical data format HDF5

- a Basis for an Emerging Standard in ICME Settings ?

G.J. Schmitz

2nd International Workshop on Software Solutions for ICME
Barcelona, Spain, 12th to 15th of April 2016

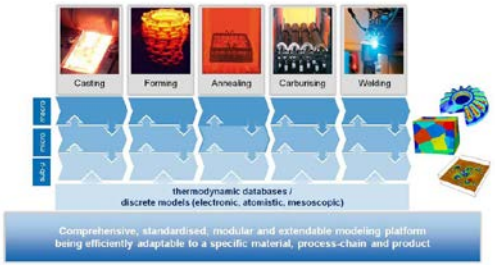
Outline

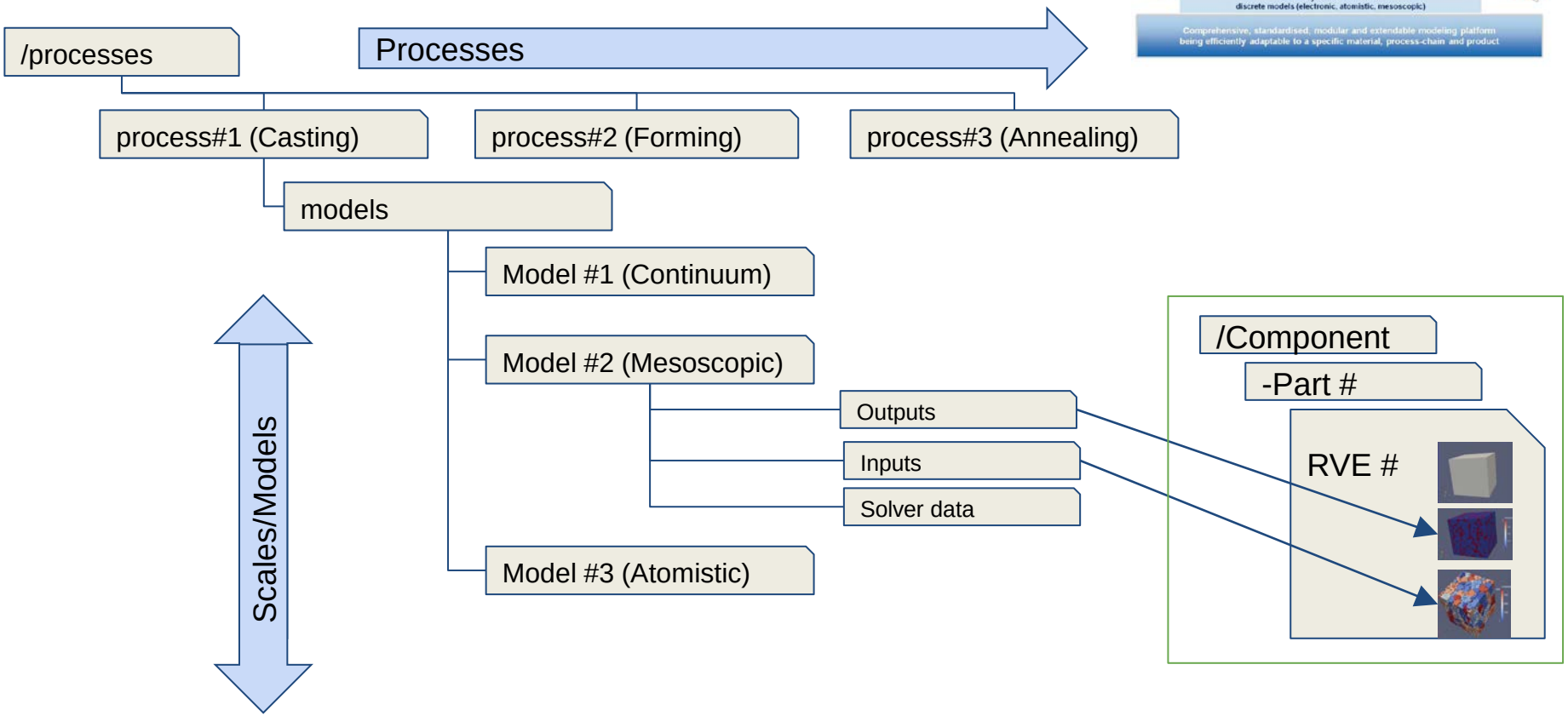
- Overall objective: create interoperability for workflows

- What is HDF5?
  - Applications of HDF5
  - HDF as a Best Practice
  - Why to use HDF5 in ICME ?
  - Main Features

- HDF Hierarchical data structure
  - Material microstructure description
  - HDF based workflow: a solution for interoperability between models

Process workflow structure

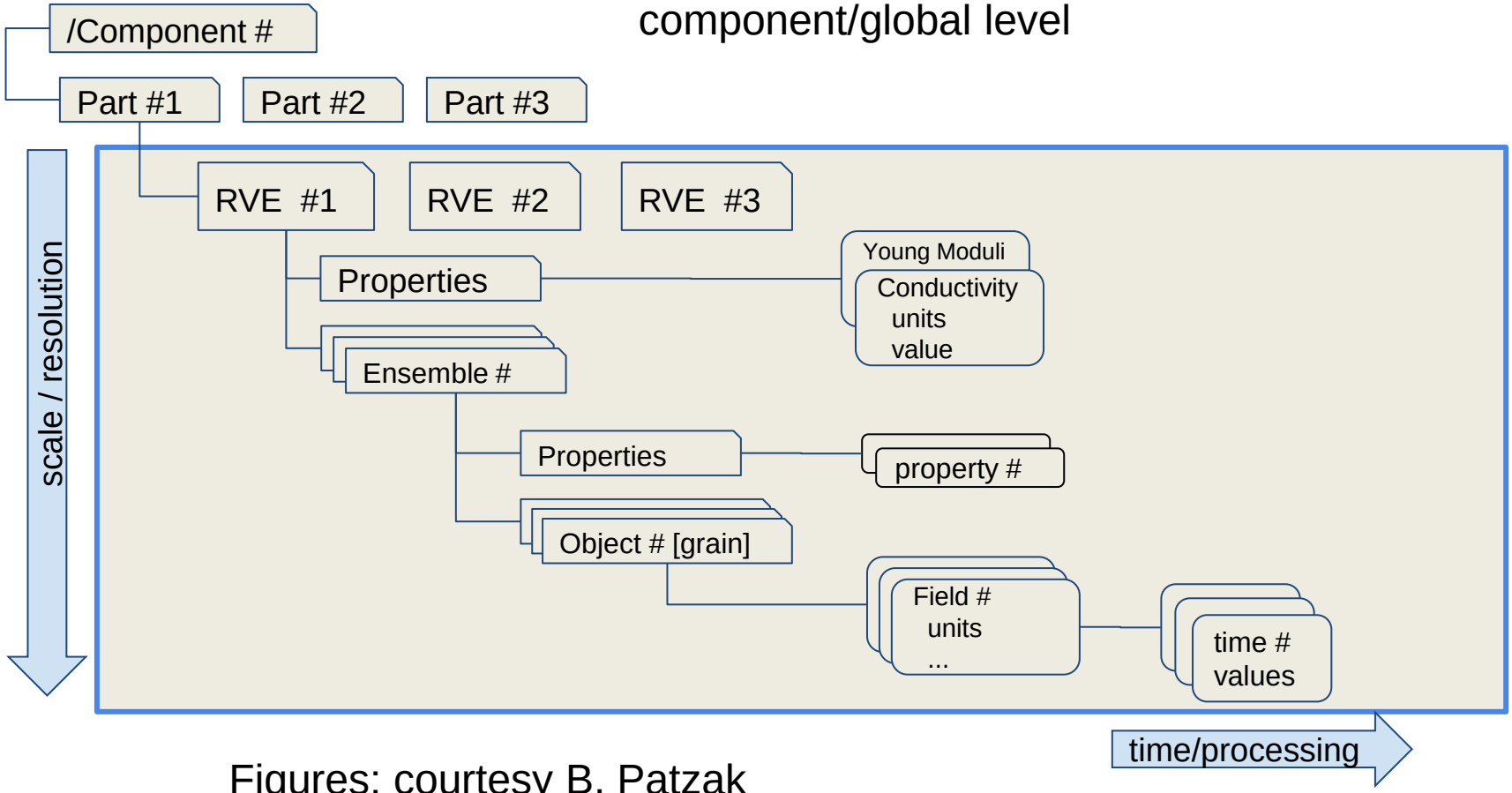




Figures : courtesy B. Patzak

Component workflow structure

RVE tracks complete history of a material point, at various scales and across processes
RVEs are included in the hierarchy starting from the component/global level



Figures: courtesy B. Patzak

Implementation of Interoperability

Objective: Interoperability

Metadata: Formal **scheme** to organize and structure data in order to establish interoperability between different types of models and different data. Metadata also allow for tracking of additional information like data about data origin, error bars, and many, many others

specific **Implementation** of interoperability and metadata schemes:

several possible solutions:

- XML
- HDF
- MongoDB
- Simple ASCII files

Topic of this talk: the widely endorsed **HDF5** based file format.

HDF5 ?

HDF software was first developed in 1987 at the National Center for Supercomputing Applications (NCSA) at the University of Illinois

What is HDF5?

The technology platform to make a difference in your relationship with large and complex data

HDF5

Hierarchical Data Format (HDF) Version 5

- Data model, file format, library, tools
- Portable, self-describing, compact
- A free and open standard

https://www.hdfgroup.org/

- A free and open source (BSD license) general purpose platform for storing, managing, archiving, and exchanging data
- Extensive facilities for data and metadata association, hierarchies, and annotation
- A self describing file format that is portable across operating systems and architectures, and that supports flexible user defined types
- A software library for high I/O performance, parallel I/O and out of core data access (partial I/O), which supports compression and other custom filters
- High quality documentation

HDF5 is best practice in numerous applications!

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Applications of HDF5

Computation
Advanced Parallel Numerical Simulation
grid computing
Machine Learning
quantum Monte Carlo

Physics
Synchrotron Science
Neutron and X-Ray Scattering
Accelerator/Plasma Science
Gas Dynamics
optical fibers
Adaptive Optics
Astronomy
AeroAcoustics
Magnetohydrodynamics
Electromagnetics,
Gravitational Waves
Remote Sensing
Scanning Near Field Optical Microscopy

Medical
design of drugs and vaccines
structure determination of subcellular complexes

Earth observation
satellite meteorology
Satellite Climate Monitoring
weather radar
Atmospheric radiation
Atmospheric Physics & Dynamical Meteorology
Ozone Monitoring

Geophysics
carbon and water fluxes modeling
land cover maps
groundwater hydrology
Biological Oceanography
fire detection
geophysics
seismic hazard analysis

Biology
DNA sequencing
bioinformatics.

mechanical engineering
Aircraft Emissions
Remotesensing
airplane engine simulation data

Electronics

Financial Engineering

HDF5 and gravitational waves

GRAVITATIONAL-WAVE DETECTOR DATA

LSC LIGO Scientific Collaboration

News | Magazine | Advanced LIGO | LIGO science | Educational resources | For

tors that were used for our GRB051103 analysis is provided here
nalysis. Any publication making use of such data should properly
We request that anyone interested in publishing anything using
t datainfo@ligo.org.
ion of this data requires careful consideration of the detector
ionary -- as well as the response of the detectors, which depends
content of the incoming gravitational wave.
ns and orie ions of the detectors, excerpted from the file
ite analy as well as some further notes and illustrations

itude s estimated at 25% for both H2 and L1 data, in
side this band). This is significantly larger than
Calibration of the LIGO Gravitational Wave
tion measurements were available from the data

- The data files can be found in this data repository.
- The data are provided in two formats: HDF5 and gzipped ascii text. Many data analysis environments can read in data from HDF5 files, including Python (see the h5py package), MATLAB, C/C++, and IDL. Links to example python scripts for reading and plotting the HDF5 files can be found below.

Length scales from light-years down to atto-meters
Time scales from billions of years to microseconds

Use of HDF5 in different software tools

ESI world-leading provider in Virtual Prototyping:
HDF5 used as data container for their new solver result database format called ERF (ESI Result Database Format)

ITK from KITWARE Inc. uses HDF5 in medical image processing.

MATLAB, one of the core products from The Mathworks, stores its data in the HDF5 format.

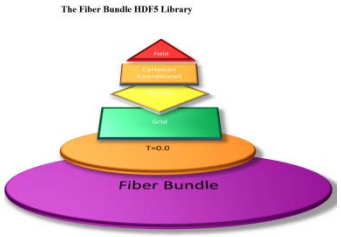
CFD General Notation System (**CGNS**)
HDF5 is standard for storage and retrieval of computational fluid dynamics (CFD) analysis data.

CFD post-processing

HDF5 and FEM

- H5Fed (HDF5 based Finite Element Data Library) defines groups and datasets as well as offers an API to read and write hierarchically structured meshes, both on serial and parallel computers. It provides adjacency relations for all topological entities of a mesh, both upward and downward. Continued within DUNE project.

- The Fiber Bundle HDF5 (F5) Library (*http://www.fiberbundle.net/*) supports structured, unstructured grids, automatic mesh refinement, Vertex-centered, edge-centered, face-centered, cell-centered data sets, scalar, vector, and tensor fields. *[Marcel Ritter, University of Innsbruck Computer Science & Civil Engineering, Introduction to HDF5 and F5, https://www.cct.lsu.edu/uploads/trs/CCT-TR-2009-13/CCT-TR-2009-13.pdf]*



HDF5 Features

https://www.hdfgroup.org/

HDF5 suite includes:

- A versatile data model that can represent very **complex data objects** and a wide variety of **metadata**.
- A completely portable file format with **no limit on the number or size** of data objects in the collection.
- A software library that **runs on a range of computational platforms**, from laptops to massively parallel systems, and implements a high-level API with C, C++, Fortran 90, and Java interfaces.
- A rich set of integrated performance features that allow for access time and storage space optimizations.
- **Tools and applications** for managing, manipulating, viewing, and analyzing the data in the collection.

HDF5 Features

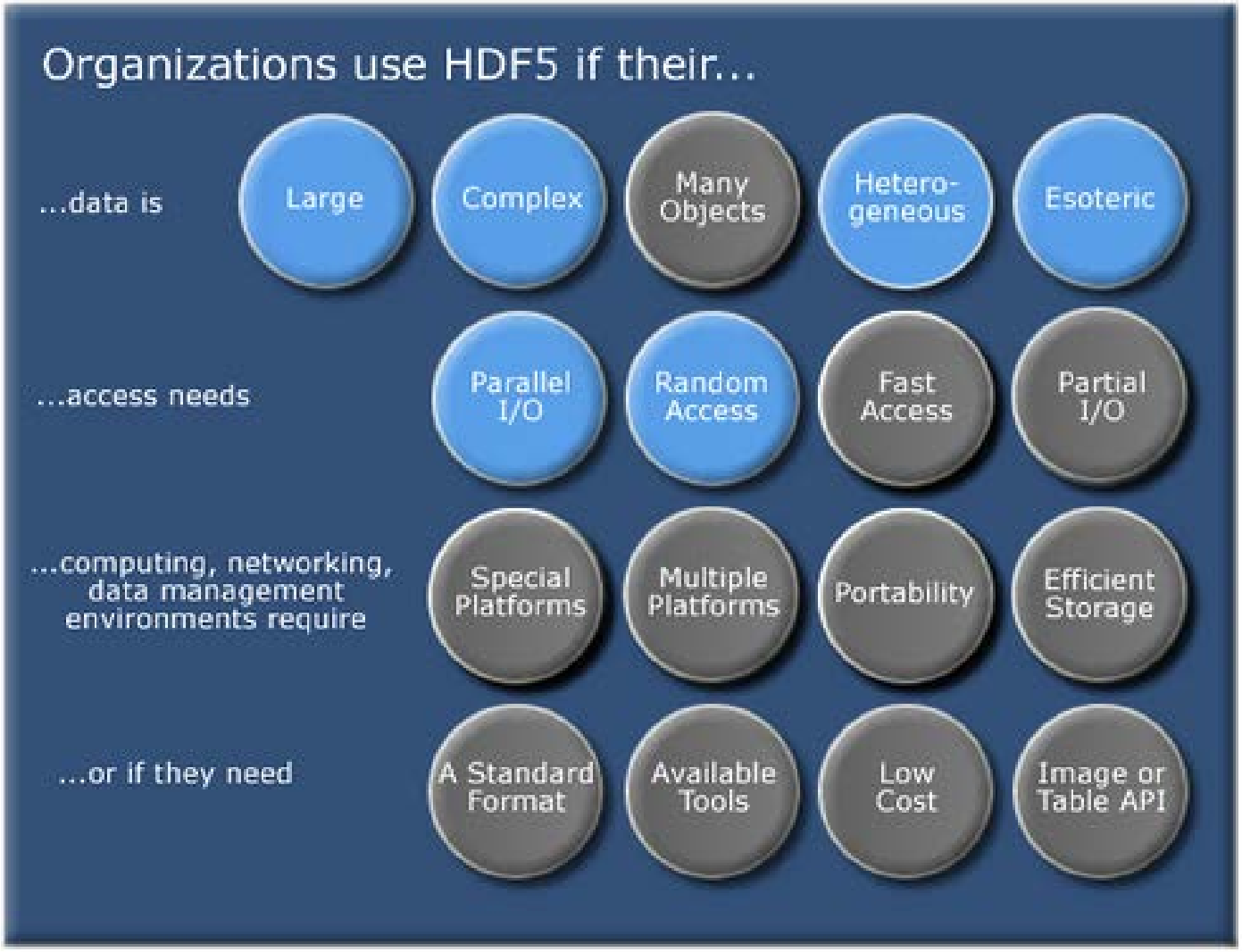
- **Free and open source**; open Format - HDF5 is widely **supported in many programs**, including open source programming languages like like R and Python,
- **Platform-independent** binary data storage with optional compression

- **Hierarchical data ordering**
- **Self-describing tags** and datasets (including metadata, no additional metadata documents)
- **"Data slicing",** or extracting only portions of the dataset as needed for analysis

- Supports **complex data relationships** and dependencies through Datasets (multidimensional arrays) and Groups (container structures)
- Different types of datasets can be contained within one HDF5 file.
- Supports Large, Complex Data: HDF5 is a compressed format that is designed to support **large, heterogeneous, and complex datasets**.

- One file can describe data from an **entire workflow**

Why use HDF5?



http://www.hdfgroup.org/why_hdf/

Why HDF for Materials Modelling?

- different models (discrete/continuum):
  - electronic, atomistic,mesoscopic, continuum
- complex and heterogenous data:

  from „positions of atoms“ up to multicomponent, multiphase, polycrystalline microstructures comprising defects
- Ease of use: inspectable by non-computer specialists similar to a windows directory
- Several applications of HDF known in experimental materials data
- Materials reveal a hierarchical structure. Need for structured data
- Much more..see this conference

Hierarchy in materials (continuum models)

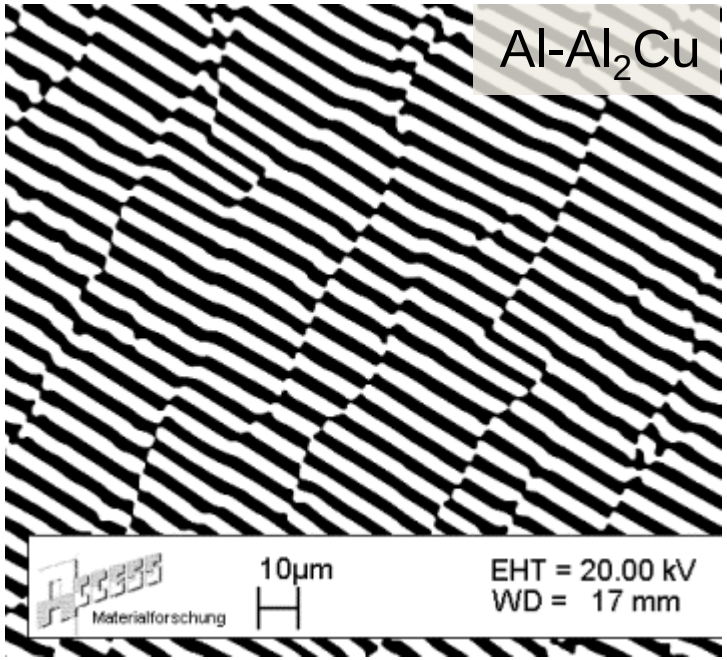
integral variables

phase fractions f_{fcc}, f_{Al2Cu}

+ state variables:
  - avrg. composition c
  - avrg. temperature T
  - avrg. pressure p

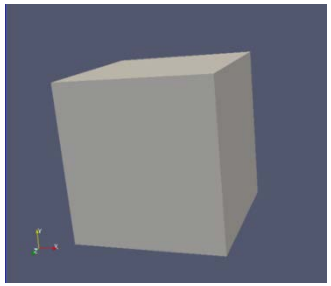
characteristic scales

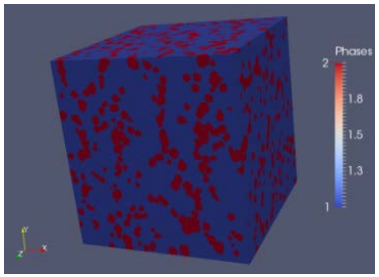
e.g. spacing λ, grain size d,

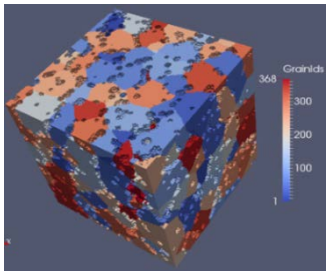


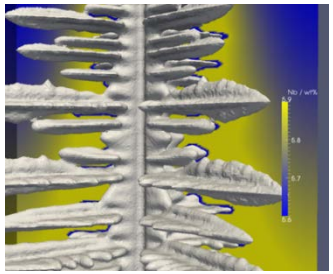
local variables

order parameter ϕ_{fcc}, ϕ_{Al2Cu}
lattice orientation o(x)
dislocation density $n_d(x,t)$
…
+ local state variables
  - local composition c(x,t)
  - local temperature T(x,t)
  - local pressure p(x,t)





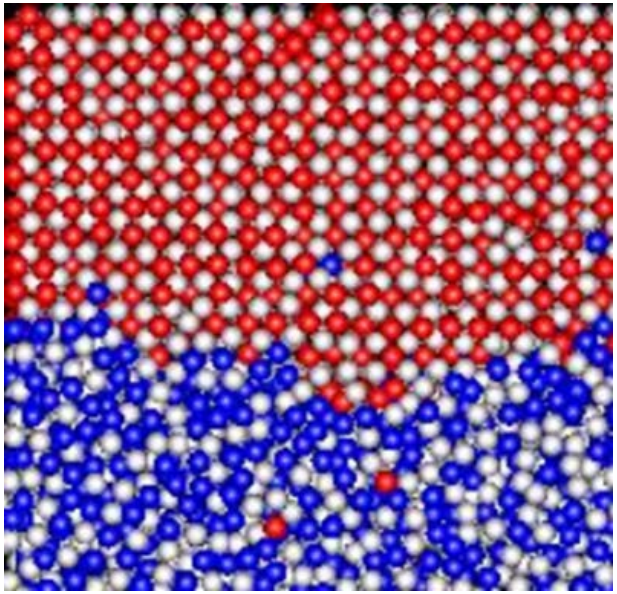




Hierarchy in materials (discrete models e/a/m)

integral variables

avrg. NumberDensity
avrg. Mass/MassDesity
avrg. composition c
avrg. vel./ temperature T
avrg. pressure p
avrg. defect density
…

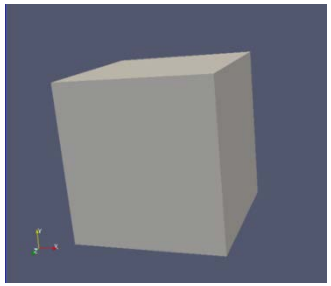


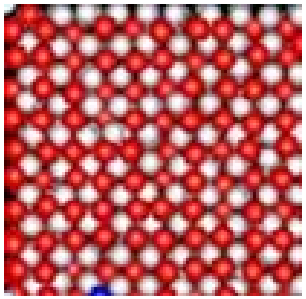
local variables

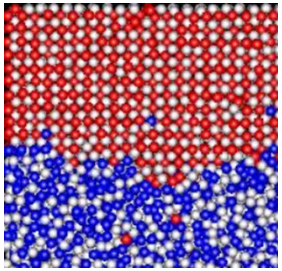
positions of atoms
velocities of atoms
types of atoms
…
…

characteristic scales

e.g. interfaces, grains, lattices, …







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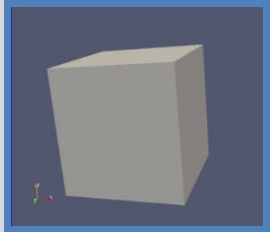
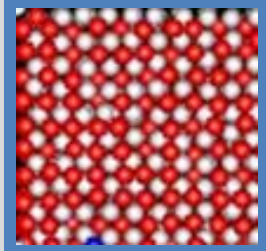
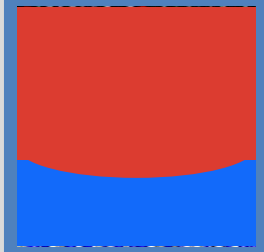
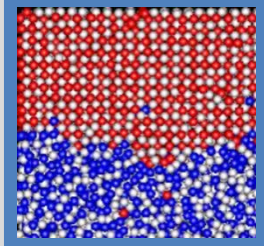
discrete (e/a/m) → continuum

e/a/m models



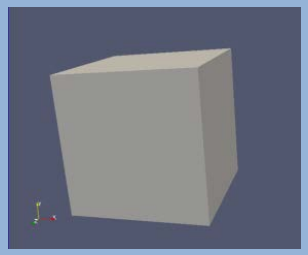


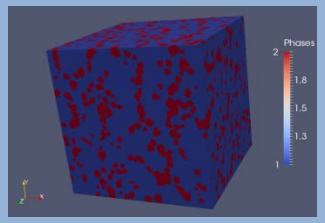


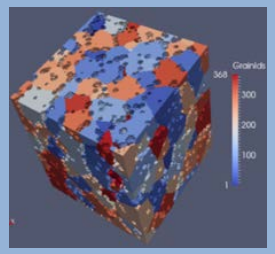


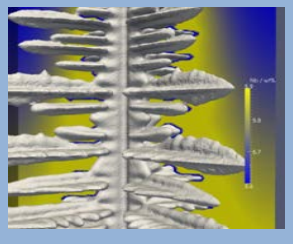
Information exchange is importatnt at ALL and even across ALL hierarchical levels !!

Inter
condu tivities, viscosities
diffusiv ties, dislocaton dynamics…









continuum models

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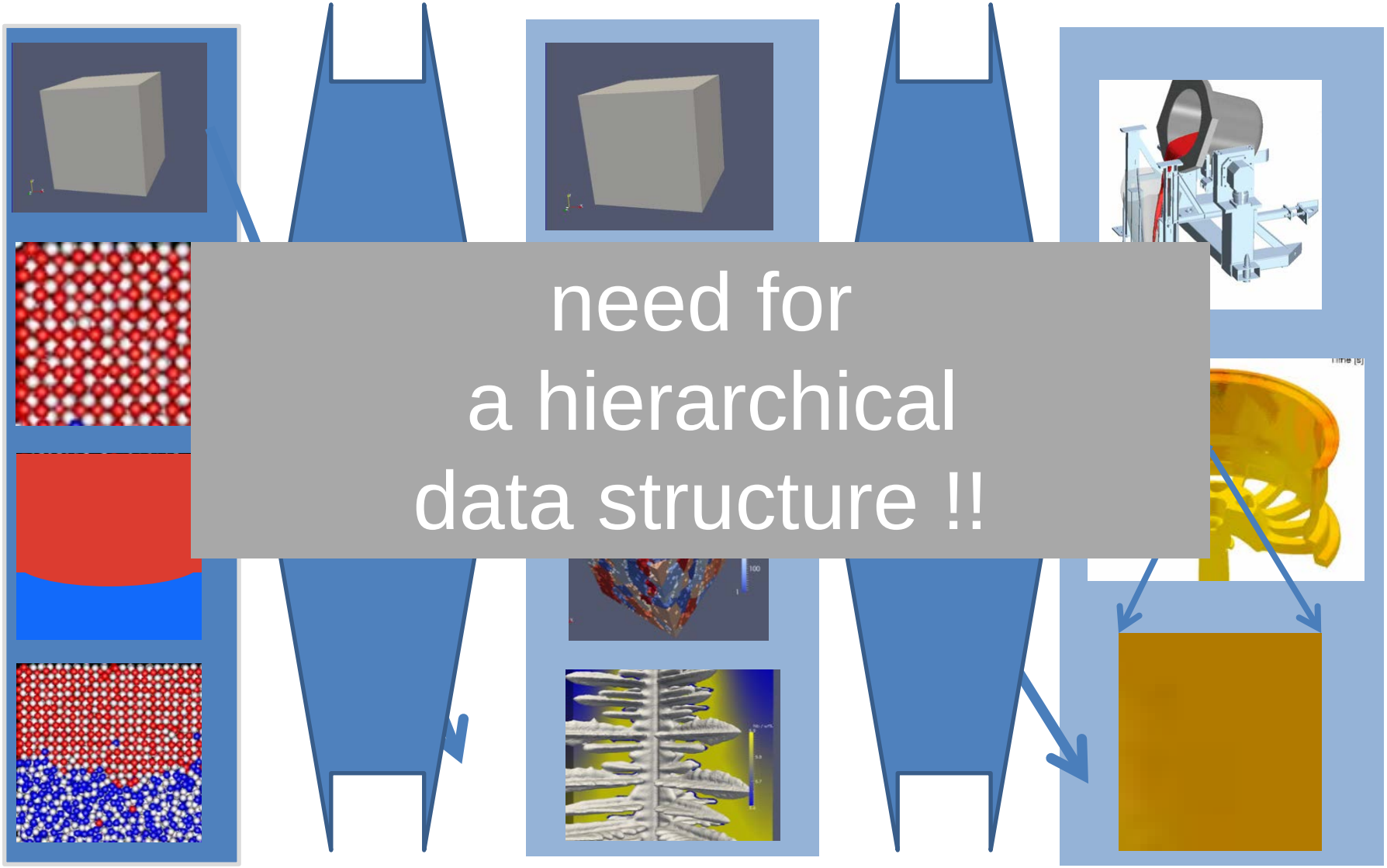
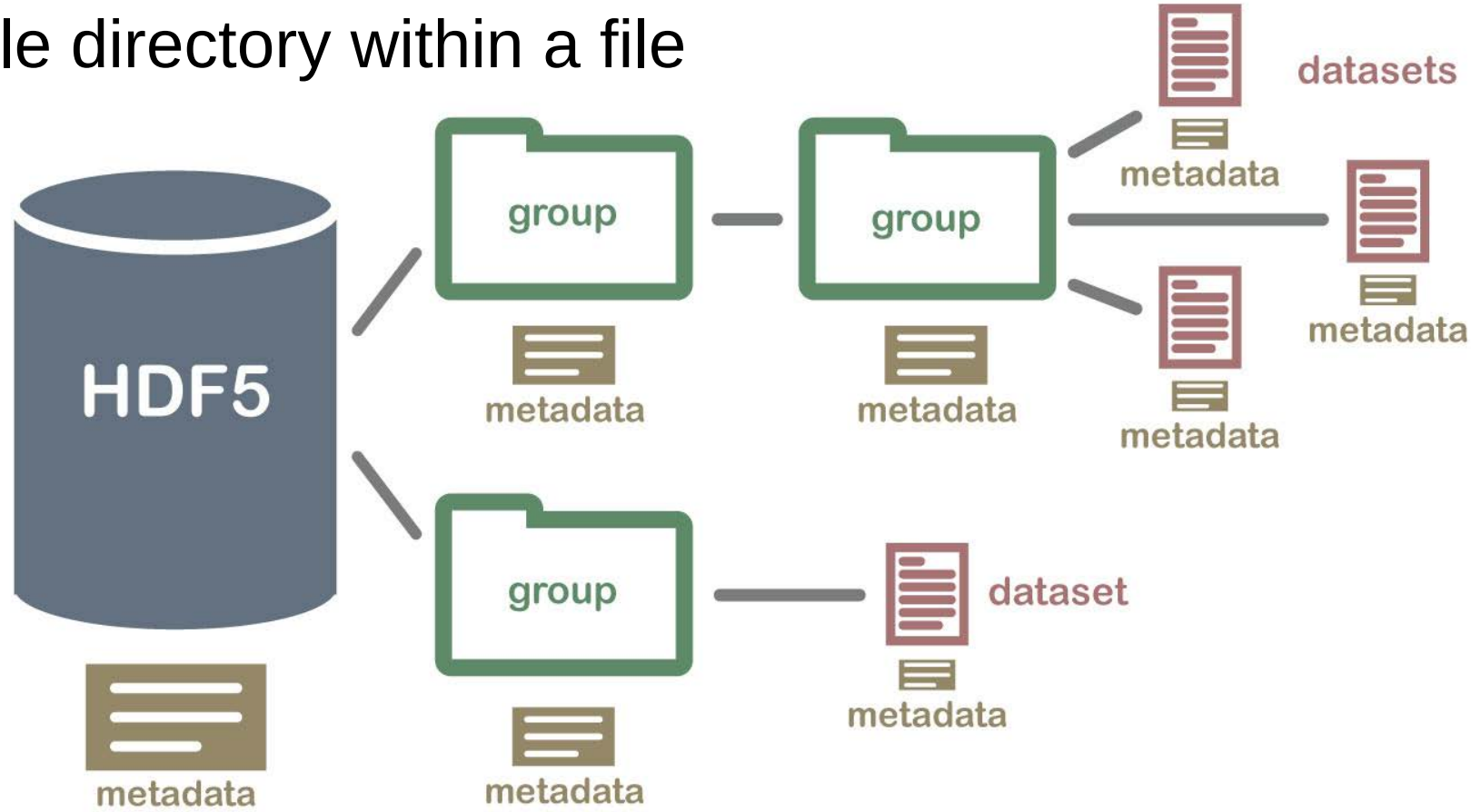
e/a/m – mesoscale continuum - macroscale



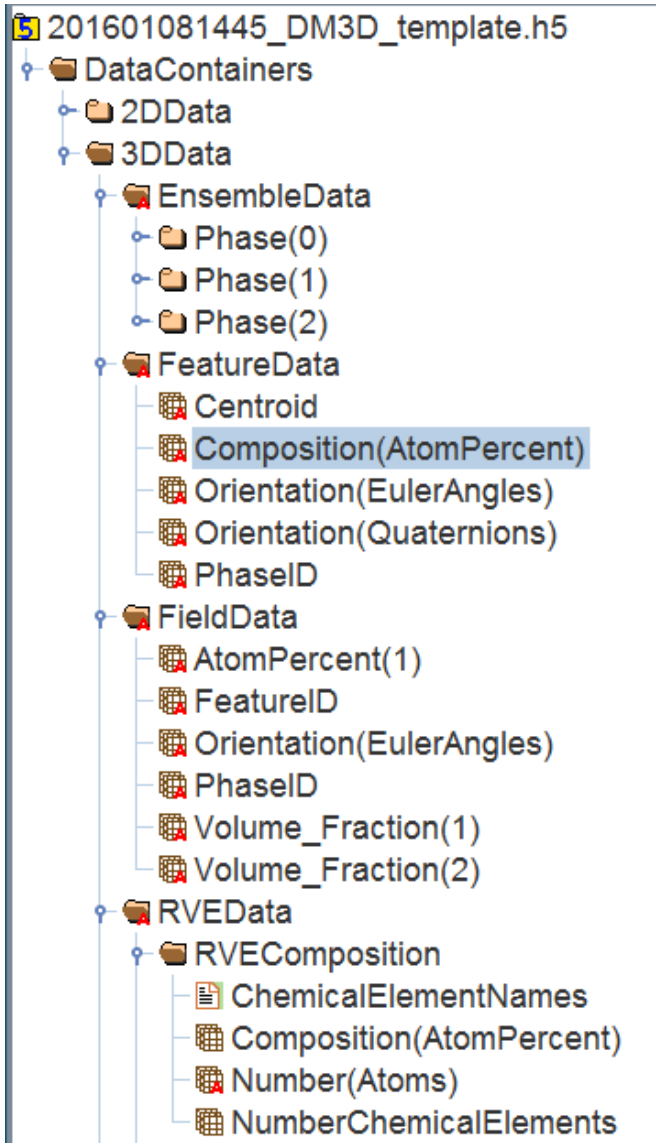
HDF5: hierarchical data structure plus metadata

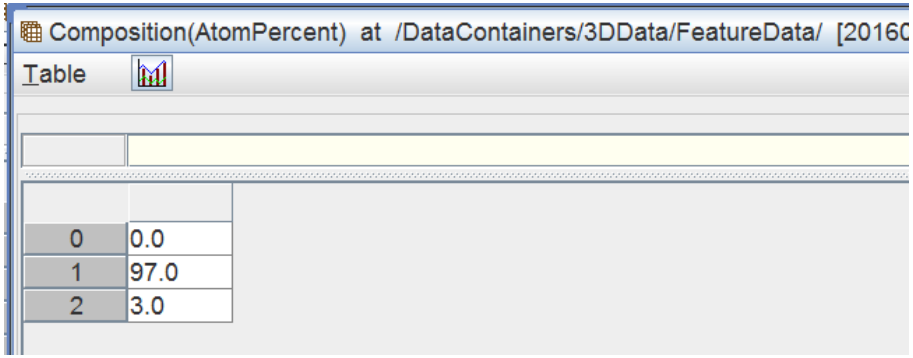
Hierarchical Structure – a file directory within a file



http://neondataskills.org/HDF5/About/

Inspecting HDF5 files with HDFview





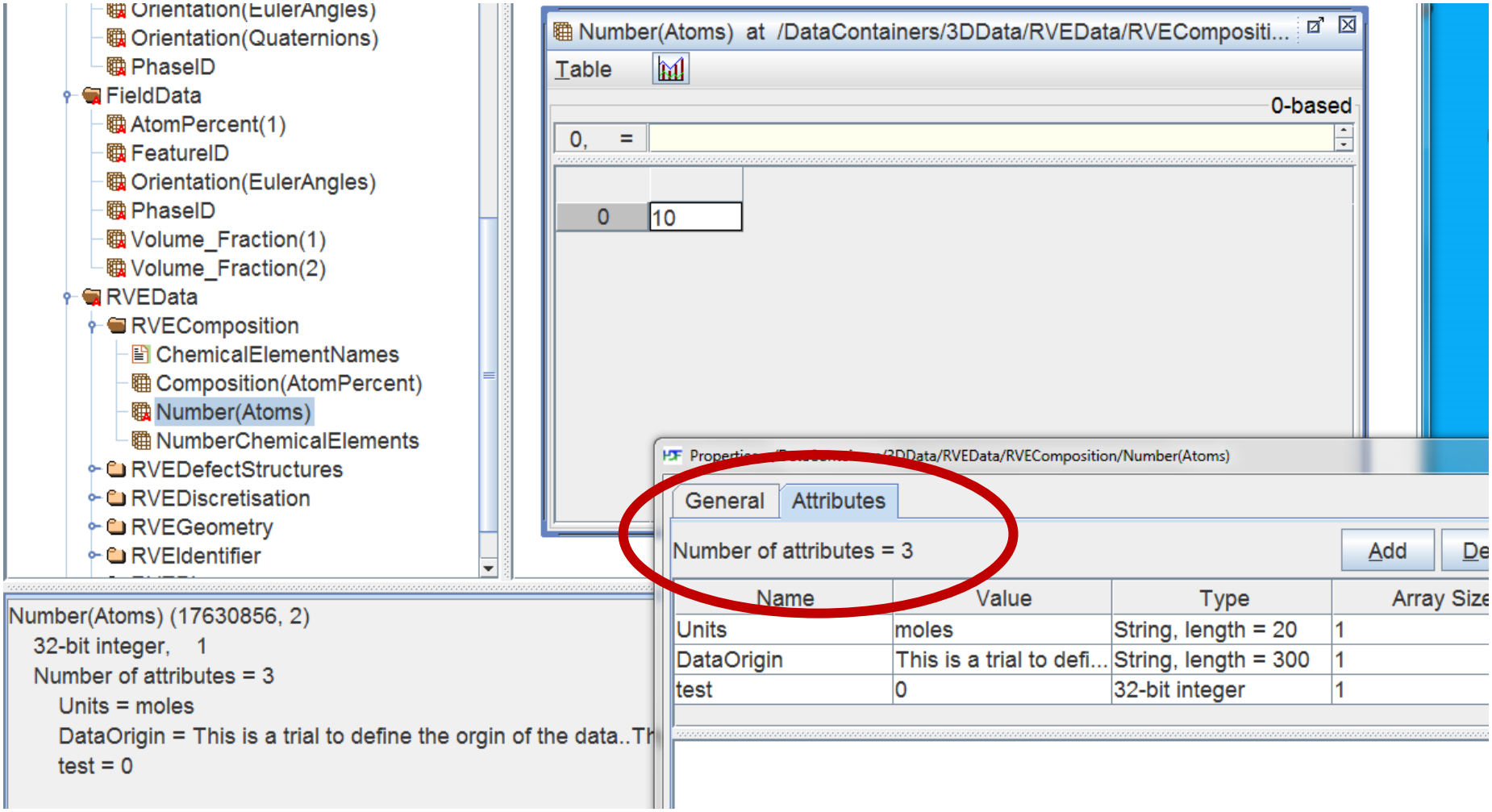
- Intuitive inspection
- similar to Windows explorer

- hierarchical structure
- extendable/amendable

- easy handling of metadata

Composition(AtomPercent) (26342560, 2)
32-bit floating-point, 3
Number of attributes = 1
Units = at._%

Handling Metadata in HDF5

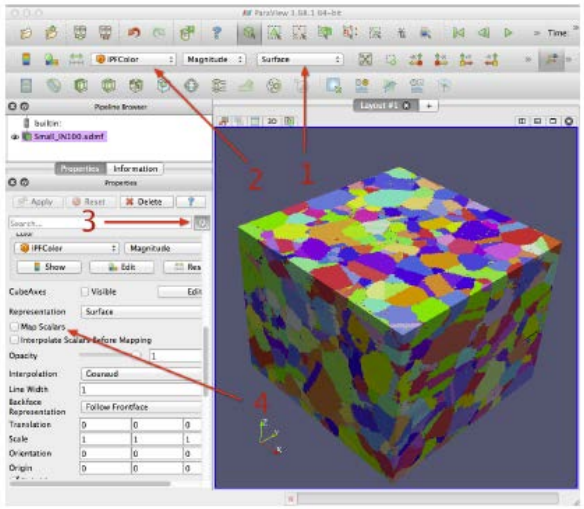


HDF5 in Materials Engineering: Dream3D

DREAM.3D (http://dream3d.bluequartz.net/)

- Collection of data analysis tools (*filters*) for the construction of customized workflows (*pipelines*) to analyze data.
- provides a flexible, extendable, and open-format data structure simplifying data exchange between collaborators

- Reconstruction of 3D microstructures from EBSD serial sectioning
- Generation of synthetic microstructures
- Algorithms available to extract various statistics like ODF, texture, neighborhood relations
- Reconstructed volumes can be exported as industry standard STL files, ParaView files (.xdmf, vtk), Abaqus (.inp).
- DREAM.3D stores all data as HDF5 files by default.



Datastructures in Dream3D

HDF5 customized to the description of materials!

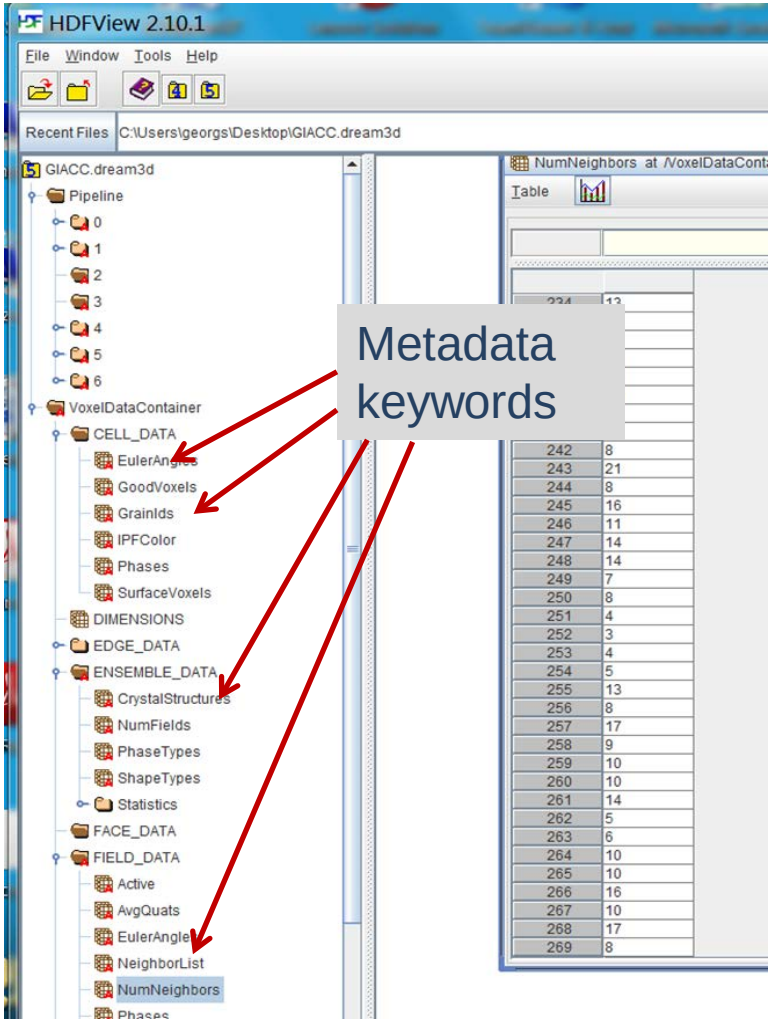
Available for :

crystallographic data per phase (simple)
Geometric information on objects
(size, shape, centroids, neighbours, …)
Orientation information on objects (Euler angles)
RVE statistics/texture
…many more

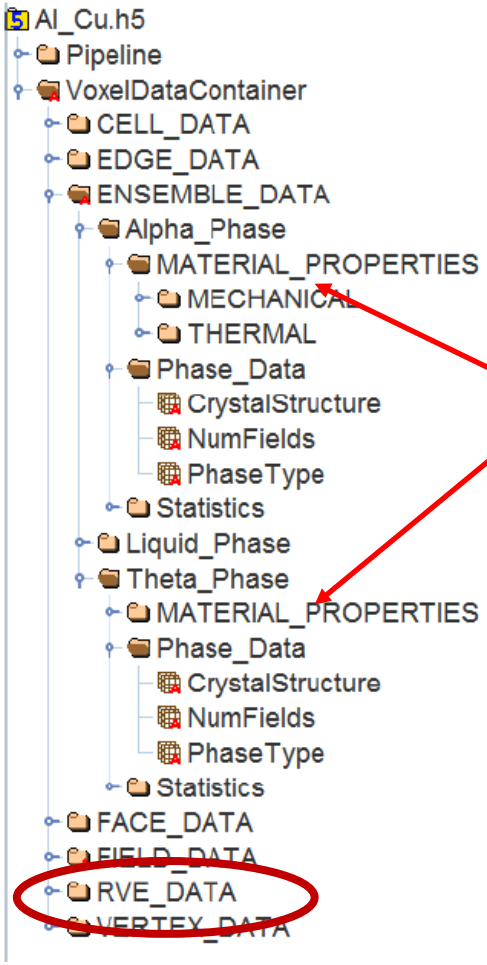
Desirable for:

- **composition data** to be included / EDX type data
- thermodynamic data to be included
- defect data to be included (dislocations etc)
- **data for properties** /elasticity/plasticity data

4D data (i.e. time dependant microstructures)



Materials description



phase containers contain properties of **each phase**

Origin of data:

- experimental
- Literature
- e/a/m models
- etc

Effective properties of the RVE being derived from knowledge about microstructure and per phase properties are stored in the MATERIAL_Properties container of the RVE data

HDF5: A New Approach to Interoperability in Finite Element Tools

A. Bhadauria, C. Agelet, M. Chiumenti and M. Cervera

Abaqus .mat file HDF5

Microstructure data for a given phase: thermodynamic, kinetic, crystallographic properties.

Material **properties for each phase** may be integrated into the **ensemble** data:

- by reading from a material file (e.g. Abaqus) for each phase
- by extracting (post-processing) such properties from discrete models. (**multiscale linking**)

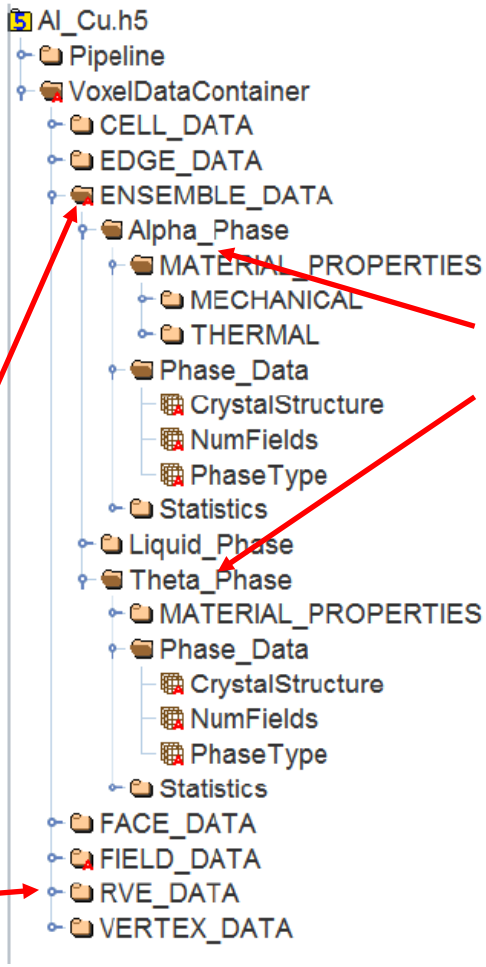
Effective properties and HDF5

Ensemble properties can be used to generate the effective properties of the RVE,

High level homogenization structure from lower scale models

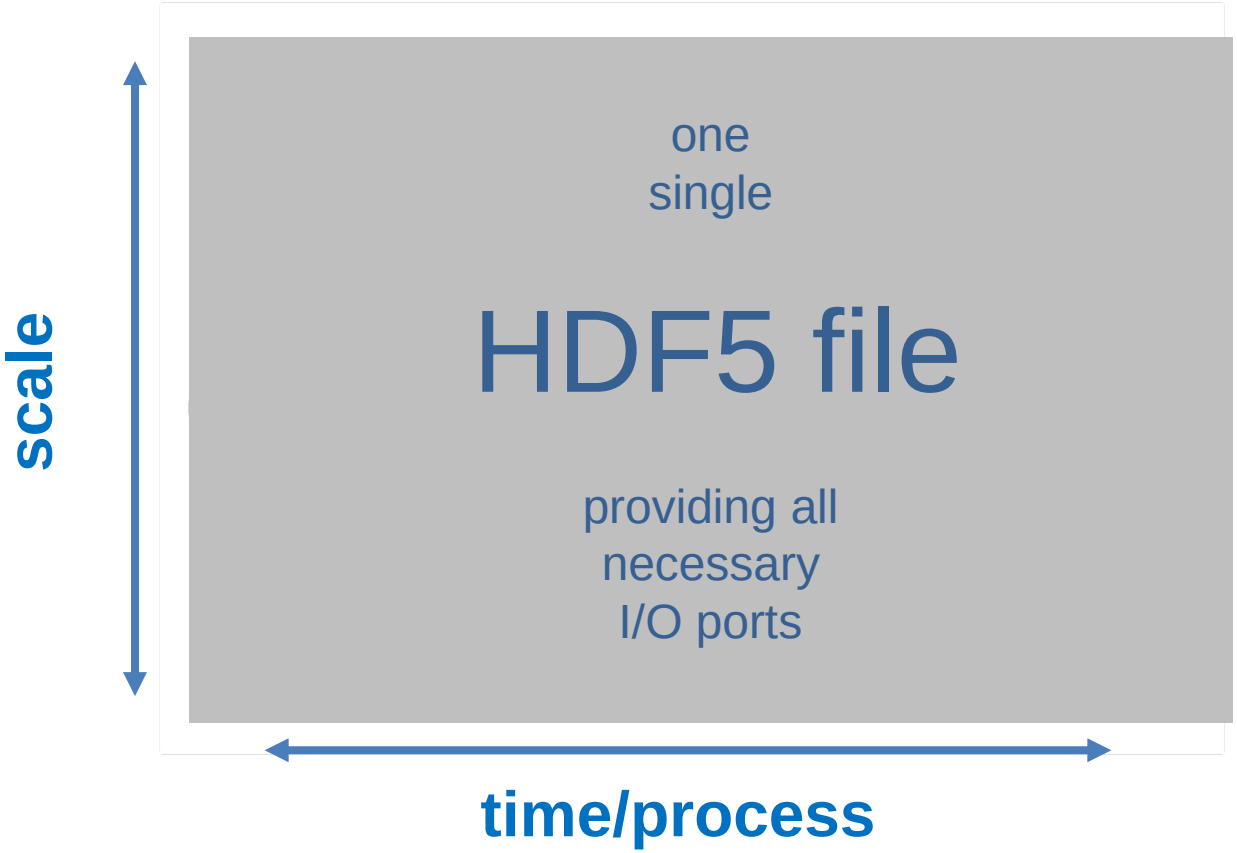
Implementation through HDF data structure:

storing **homogenized properties** at different hierarchical **levels** in the **same** data structure.



phase containers containing all properties of a phase

Information flow between material models



Basic scheme of a simulation workflow. **Linking of models**:

- Along the **time/history**: from initial conditions to output/final conditions
- Across the **scales** via exchange of **boundary** conditions and **effective** values

Need for metadata descriptors

Towards a Metadata Scheme for the Description of Materials

-the Description of Microst[illegible]es-

G.J.Schmitz, B.Böttger, M.Apel, J.Eiken, G.Laschet, [illegible] .Berger, G.Boussinot, A.Viardin

- to appear in „**Science and T[illegible]gy of Advanced Materials**" (under review)
- scheduled t[illegible] in spring 2016 on-line as open access
- HD[illegible]plate file comprising the defined descriptors will be provided along with publication

see also talk in Session 7B

Conclusions

- HDF is established as a “best practice” in many areas of application
- HDF has been presented as a possible choice for data storage/implementation level for interoperability
- HDF hierarchical data structure allows for a description of an entire workflow in a single data file
- All processes and models in the workflow can operate on the shared component/material data structure
- The HDF data structure allows homogenization of material properties as it contains both local and integral data

Benefits of HDF hierarchical data structure

- Store and retrieve information at the desired level of detail
- allows integration of information from all types of sources/models (also experimental!)
- Selected parts of the file can be exchanged individually
- Meets the hierarchical structure of materials

HDF may become a hub for information exchange between models (electronic/atomistic/mesoscopic/continuum)

HDF5 during THIS workshop (explicit)

The Hierarchical Data Format HDF5 - a Basis for an Emerging Standard in ICME Settings?
Georg J. Schmitz

HDF File-based interoperability for multiscale modelling
Fabio Sacconi and Stefano Bellocchio

On the usage of HDF5 in the DAMASK crystal plasticity toolkit
F. Roters, C. Zhang, P. Eisenlohr and P. Shanthraj

HDF5: A New Approach to Interoperability in Finite Element Tools
A. Bhadauria, C. Agelet, M. Chiumenti and M. Cervera

Thermodynamics and HDF5: Towards a Metadata Keyword Scheme for the Description of Thermodynamic Properties
S. Petersen

HDF5 during THIS workshop (implicit)

Database concepts and ICME links for atomistic simulations
Joerg Neugebauer

Implementation, benefits and handling of formal metadata schemata as enablers for Platform interoperability - From Data Structures to Modelling Platforms
T.F. Hagelien, A. Hashibon and S. Amini

Role and Descriptions of Chemical Element Distributions in Microstructure Simulation
B. Böttger and J. Eiken

Organization of materials data for efficient ICME implementation
A. Salem, J. Shaffer, R. Kublik and D. Satko

Towards a Metadata Keyword Scheme for the Description of Materials – Keywords for the Description of Microstructures –
Georg J. Schmitz, Bernd Böttger, Markus Apel, Janin Eiken, Gottfried Laschet, Ralph Altenfeld, Ralf Berger, Guillaume Boussinot and Alexandre Viardin

The Distributed and Unified Numerics Environment (DUNE)
Oliver Sander

Creating a Common Environment for Storing, Sharing and Working With Digital Microstructure Data: Thoughts and Lessons Learned
Michael Groeber, Michael Jackson and Sean Donegan

HDF5 !! — seems interesting to me (us) !!

The HDF Group

HDF software was first developed in 1987 at the National Center for Supercomputing Applications (NCSA) at the University of Illinois

Integration of e/a/m data and continuum data structure

Geometry/structure:

lattice vectors, position, atomtype, material name, composition, strain

Properties

– **Mechanical**

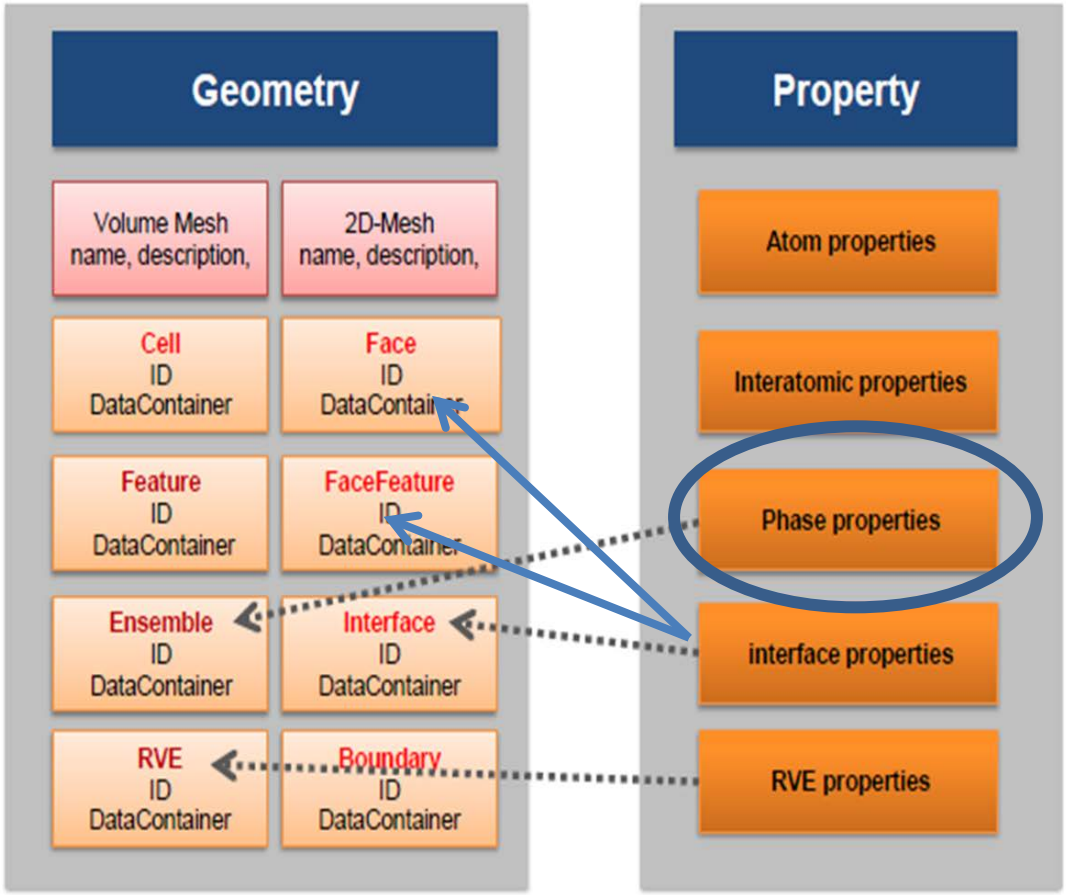
piezoelectric coefficients, elasticity

– **Electronic**

Bulk: Band gap, Band gap bowing, Valence band offset

Band structure: effective mass, band energy, alpha, deformation potentials

Total energy of the system from the DFT calculation (*Hamiltonian*)



Solver parameters:

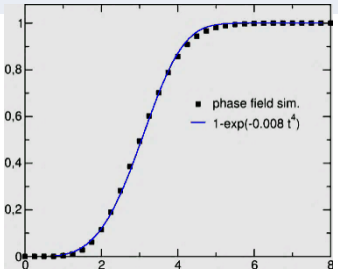
TB parameters, k•p (Luttinger) parameters, internal strain parameters, VFF parameters

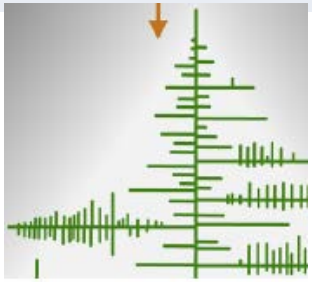
Process description

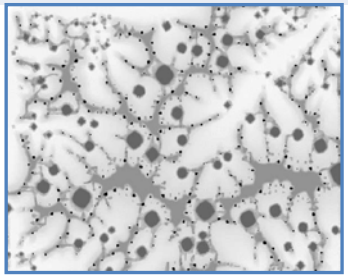
- 4D data, i.e. time-dependent microstructures, could be thought of as a sequence of HDF5 files
- All spatially resolved data could be described in vtk only
- Description of phase data,, RVE effective properties etc. through HDF5 structures (with vtk describing All spatially resolved data being something like a subset)
- Description of Workflows and temporal evolution of materials through combinations of HDF5 (and other data and file types) and probably best achieved on the basis of xdmf (with HDF5 being a subset)

Hierarchy of models

integral models p = f(t)	intermediate p = f(t,λ)	comprehensive models p = f(t,x)
thermodynamics + relaxation	CAFE	Monte Carlo Potts model
Scheil-Gulliver	needle crystal	phase field / phase field crystal
JMAK kinetics	precipitation/ripening (LSW)	cellular automaton
volume averaging	envelope dynamics	level set
…		lattice Boltzmann
		…







increasing fidelity and number of variables

Outline

- What is HDF5?
  - Applications of HDF5
  - Use of HDF5 in software tools
  - HDF for FEM
  - Features
  - Hierarchical data structure

- Motivation: Why we need a hierarchical data structure
- HDF for microstructures
  - Hierarchy in description of materials
  - Application: Dream3D
  - Example of data structure
  - Data flow for Multiscale approach

Benefits & Drawbacks of HDF5

Benefits

- hierarchical data format with metadata support
- portable (endianess) and flexible file format and a API to store or retrieve multidimensional arrays,
- data model is defined in the file
- parallel I/O implementation (Array data transfer can be collective or independent.)
- Interface to C/C++/Fortran/Java/Python/Matlab/CLI/...
- de facto standard (netCFD also can use HDF as storage format)
- Open visualization tools suporting HDF (Paraview)

Drawbacks

- Openness: For commercial applications, data encryption is often imperative.
- No existing widely accepted HDF standard in FEM community