

# Three roles of materials information for material science

Kohmei HALADA

Invited senior scientist, National Institute for Materials  
Science

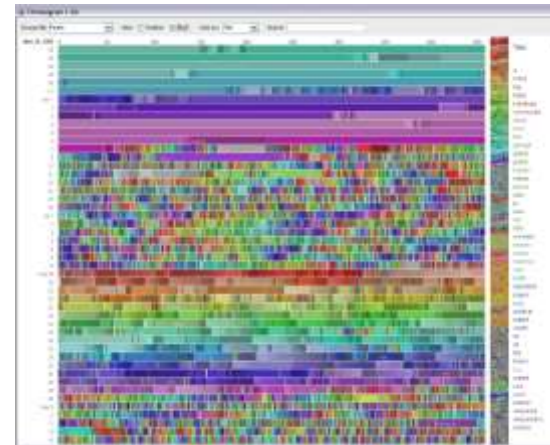
Member of committee on data center, international data  
science section, Science Council Japan

- Materials information provide researchers and developers three data spaces and coordinates, namely virtual space, material space, social space. As virtual space may be discussed well in this meeting, This presentation mentions about remaining two spaces. Social coordinate gives incentive of research and sequentially leads to out-reach of the result. The Strategic Element Initiative is a good example which was given the motivation from materials social data. Material space is the space where researchers work mainly until now. New waves is occurring in this space. The data of material itself has 4 dimensions including time, and archive time dimension comes aboard adding to them. However, we have described and transported data on only two dimension space as paper until now. “Open data” and “Data journal” are opening new world.

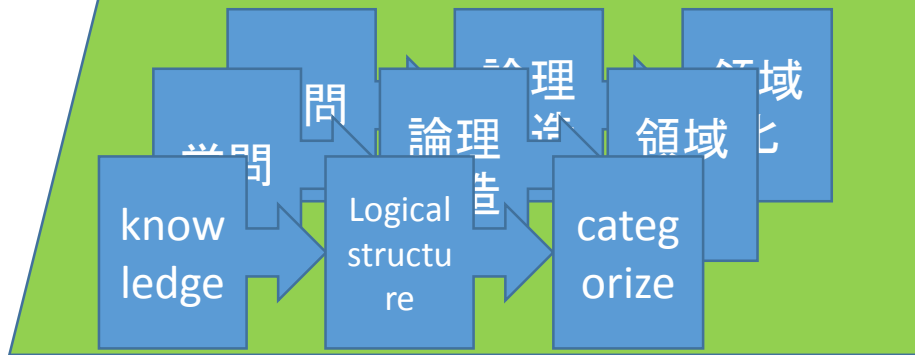
3. Dr. Masanori Kohyama , AIST, Kansai, Japan, “*Ab initio* total energy and local stress : informatics perspective”
4. Dr. Satoru Yamamoto, *BIOVIA*, Japan, “Strategy to Accelerate Material R&D- Material Informatics & Multiscale Modeling”
5. Prof. Yutaka Oya , Tohoku University, Japan, “Multidisciplinary optimization of epoxy resin based on molecular dynamics simulation”
6. Dr. Halada, Kohmei, NIMS, Japan, “Urgent Subject of Materials Informatics is How to Construct Bigdata for Materials Science”
7. Dr. Kwang-Ryeol Lee, KIST, Korea, “Development of Nano Materials Design Platform Based on Multiscale Materials Modeling”

# Big data

- Definition: Huge or complicate data which cannot treat by existing software nor application to collect, select, storage, and manage.
- Why huge
  - live-data (2.5exa bit data /day/person are created.)
  - enormous open platform
- Why complicated
  - diversity of aims and interpretations



# Connect the disciplines: informatics



Informatics is a window into this dynamic relationship, examining the interplay of people and technology **University of California, Irvine**

「application of information to artistic, science and human」and  
**University of Indiana** 「to innovation of social」

The study of the structure, the behavior, and the interactions of natural and engineered computational systems. **University of Edinburgh**

Business or law without the barrier of information

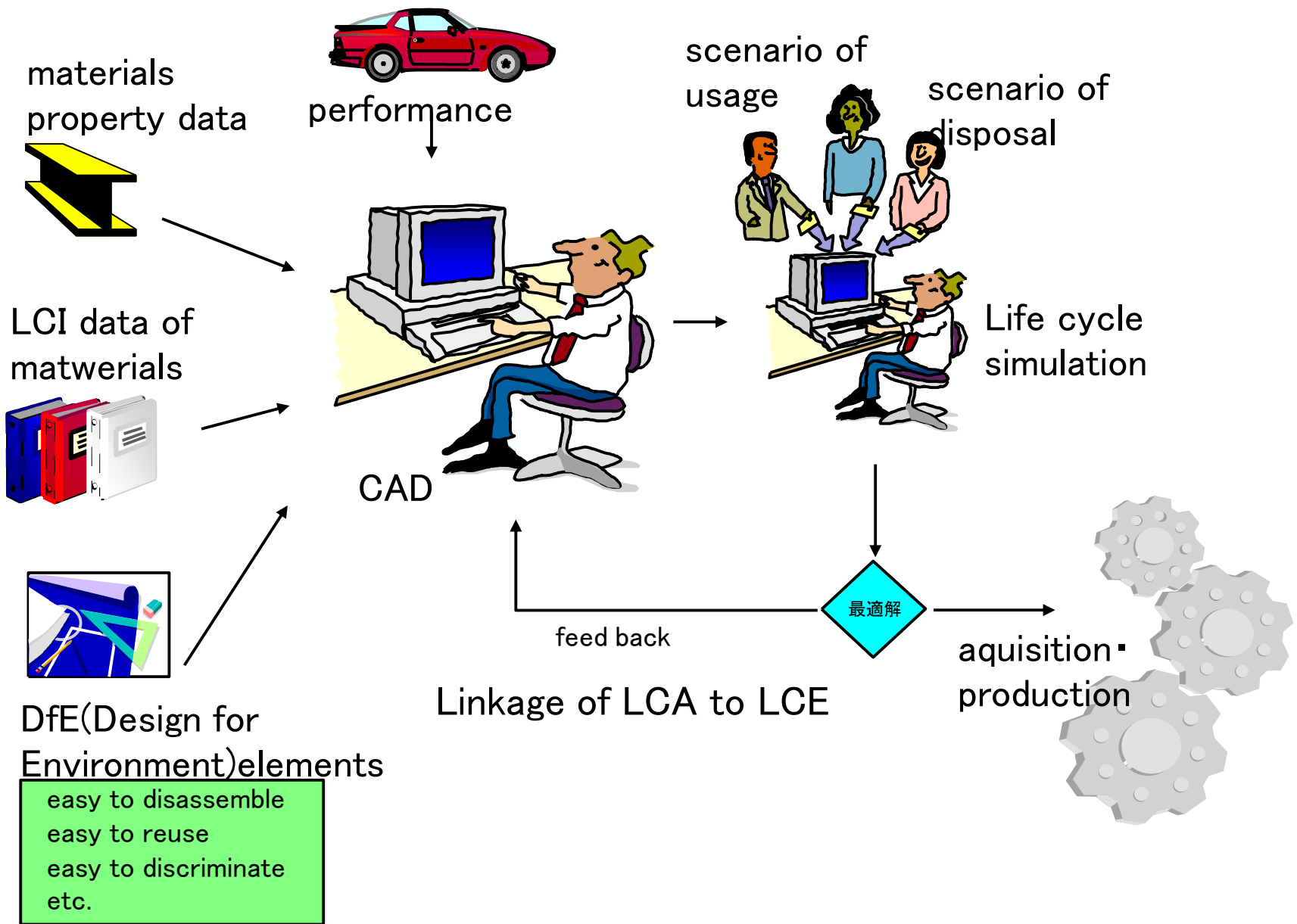
Digital technology by computer

Study on the expression, processing and communication of information

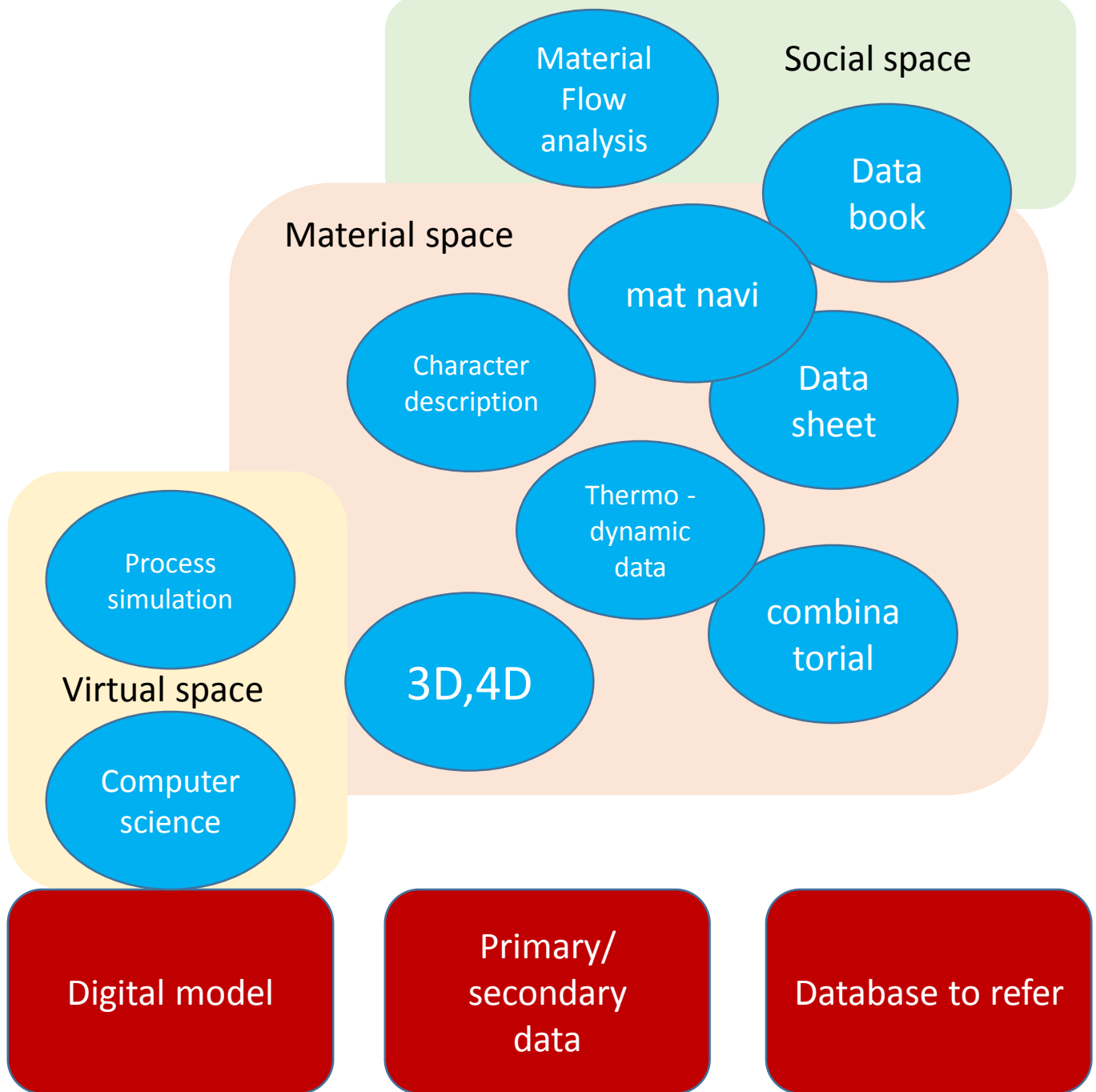
Computer science

Informatics: inter-disciplinal area which deal with the results and the structure of information.

communication



Accepters of information



Action of informatics

# Are we ready to use big data?

- **Social space** : **optimistic**

Medium size live data are open to be analyze from different view point.

Data analysis effects strategy of development.

Socio-economic data are growing day by day

- **Material space**: **pessimistic**

Almost data are not open.

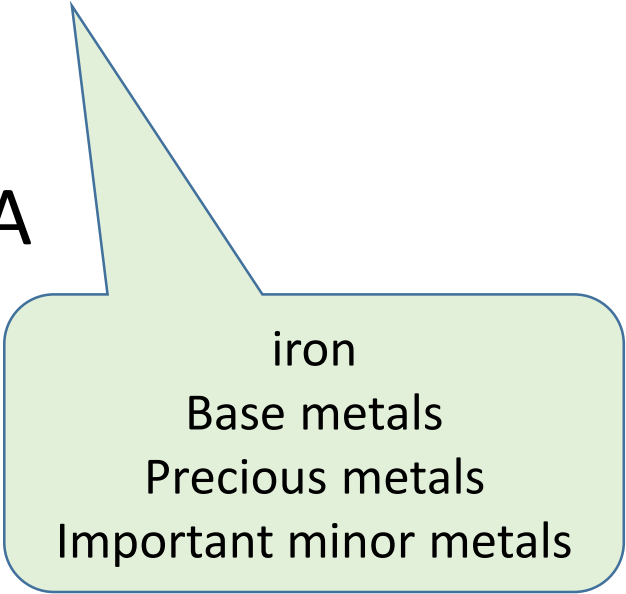
Treatment is enclosed in each discipline.

Common platform is not developed.



# Historic Move of Current Global Flow of Strategic Metals

Kohmei HALADA



- iron
- Base metals
- Precious metals
- Important minor metals

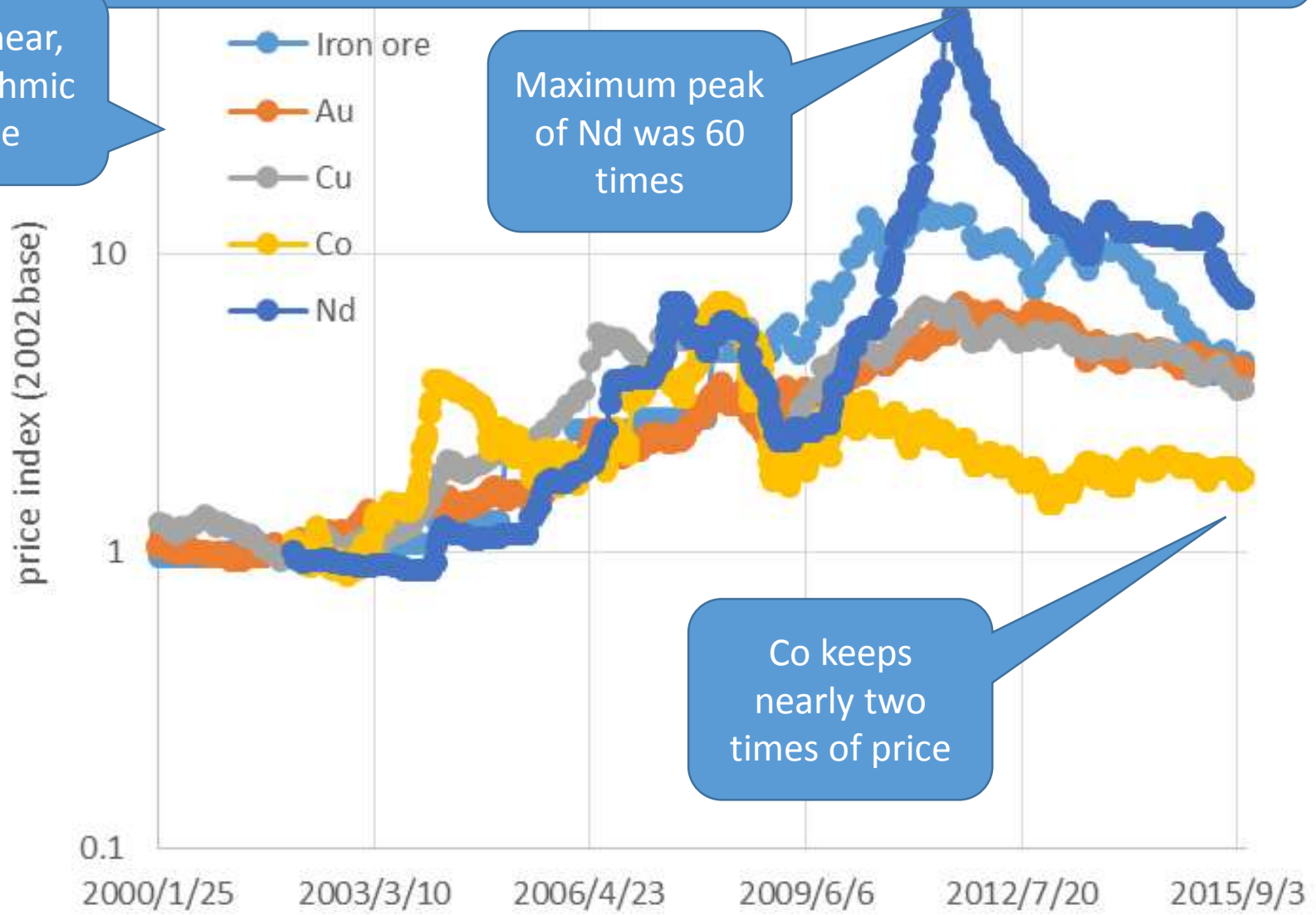


Prices have changed more drastically

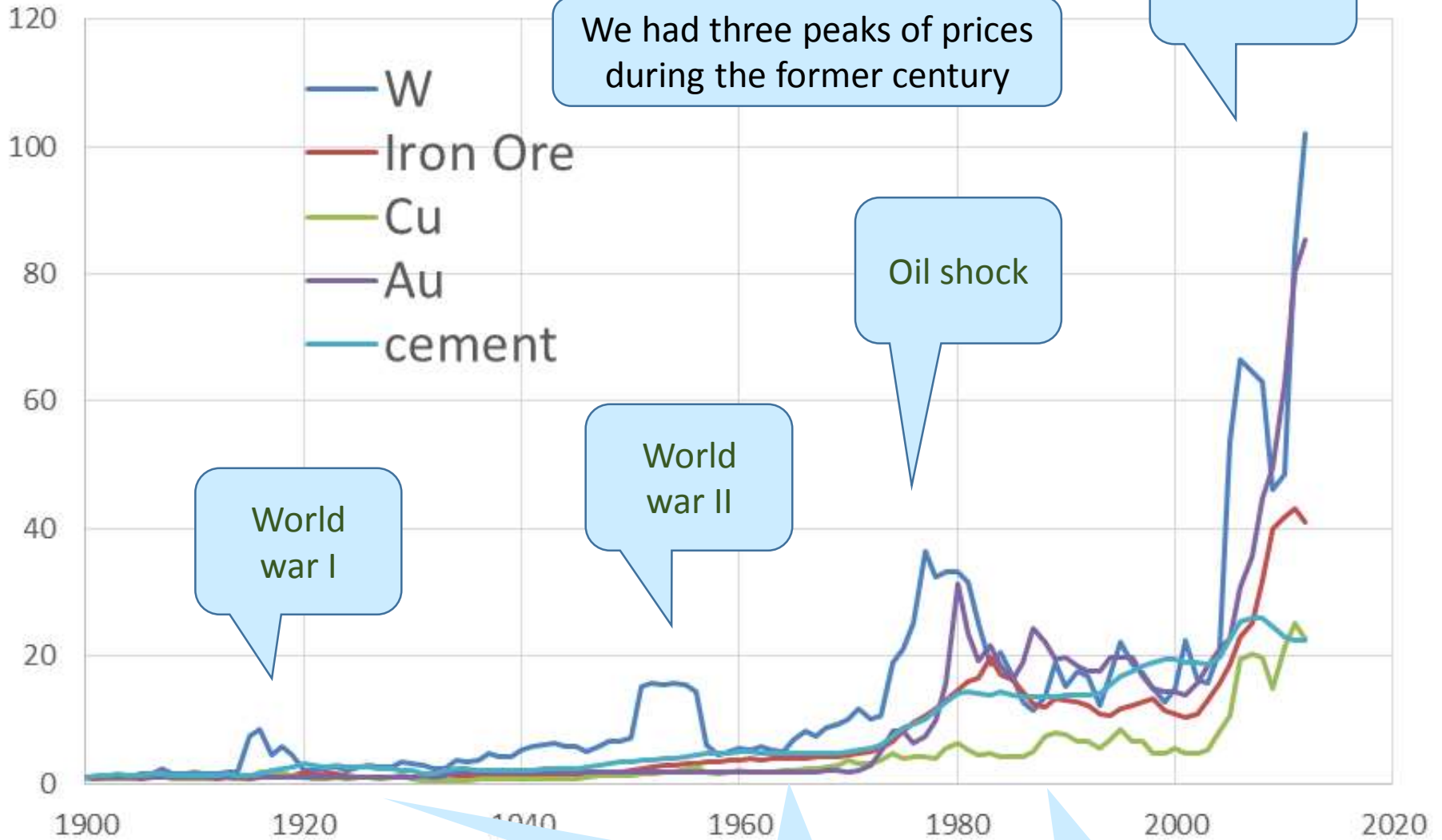
Not linear,  
Logarithmic  
scale

Maximum peak  
of Nd was 60  
times

Co keeps  
nearly two  
times of price



# Historical resource price from 1900



We had three peaks of prices during the former century

now

World war I

World war II

Oil shock

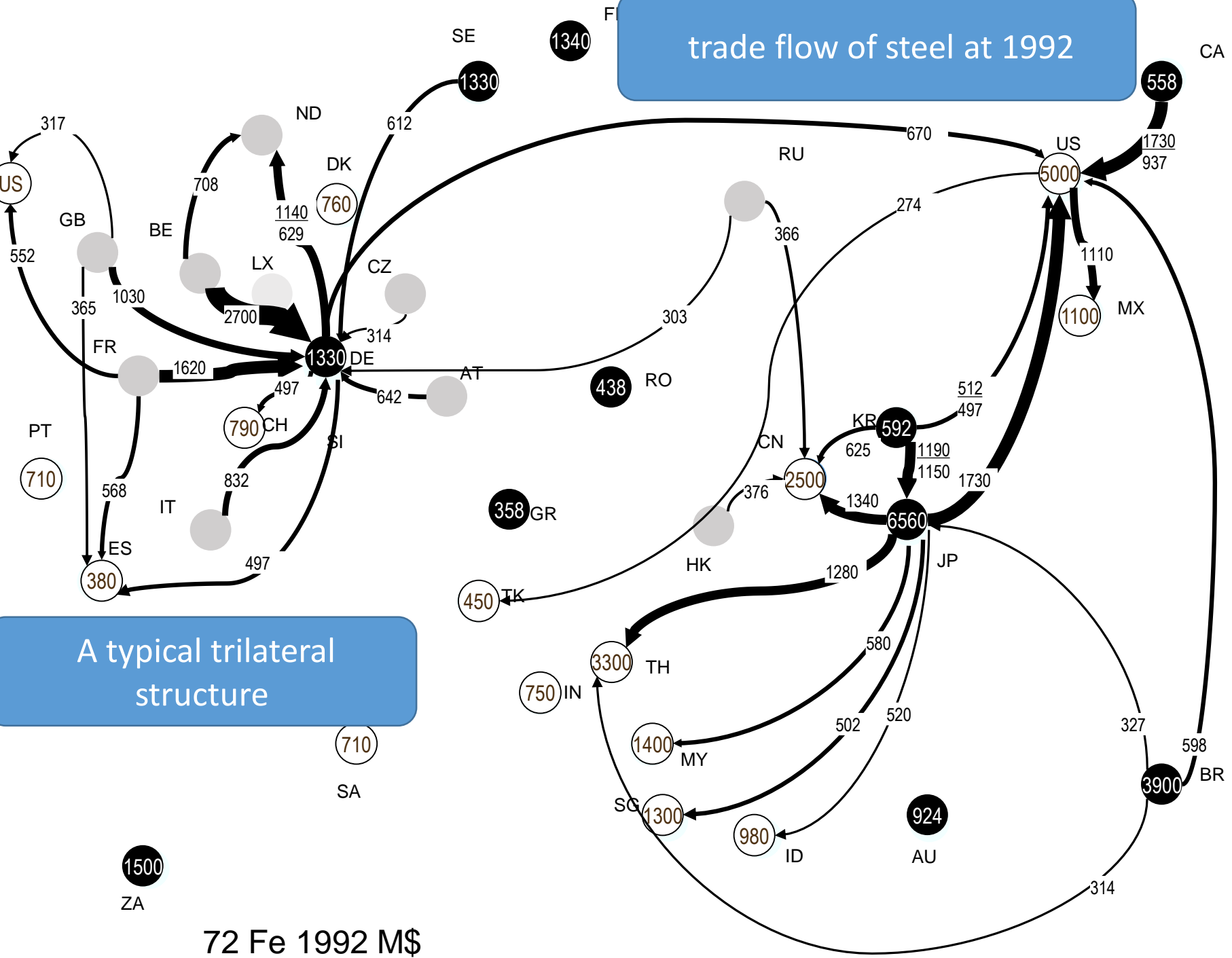
After the peak, prices shifted higher levels

What is happening ? What will come after?

Shift from the structure of the 20<sup>th</sup> century  
to the 21<sup>st</sup> century.

From **trilateral structure** of EU, US, JP  
to *universal power economy* through “**the  
factory of the world**”

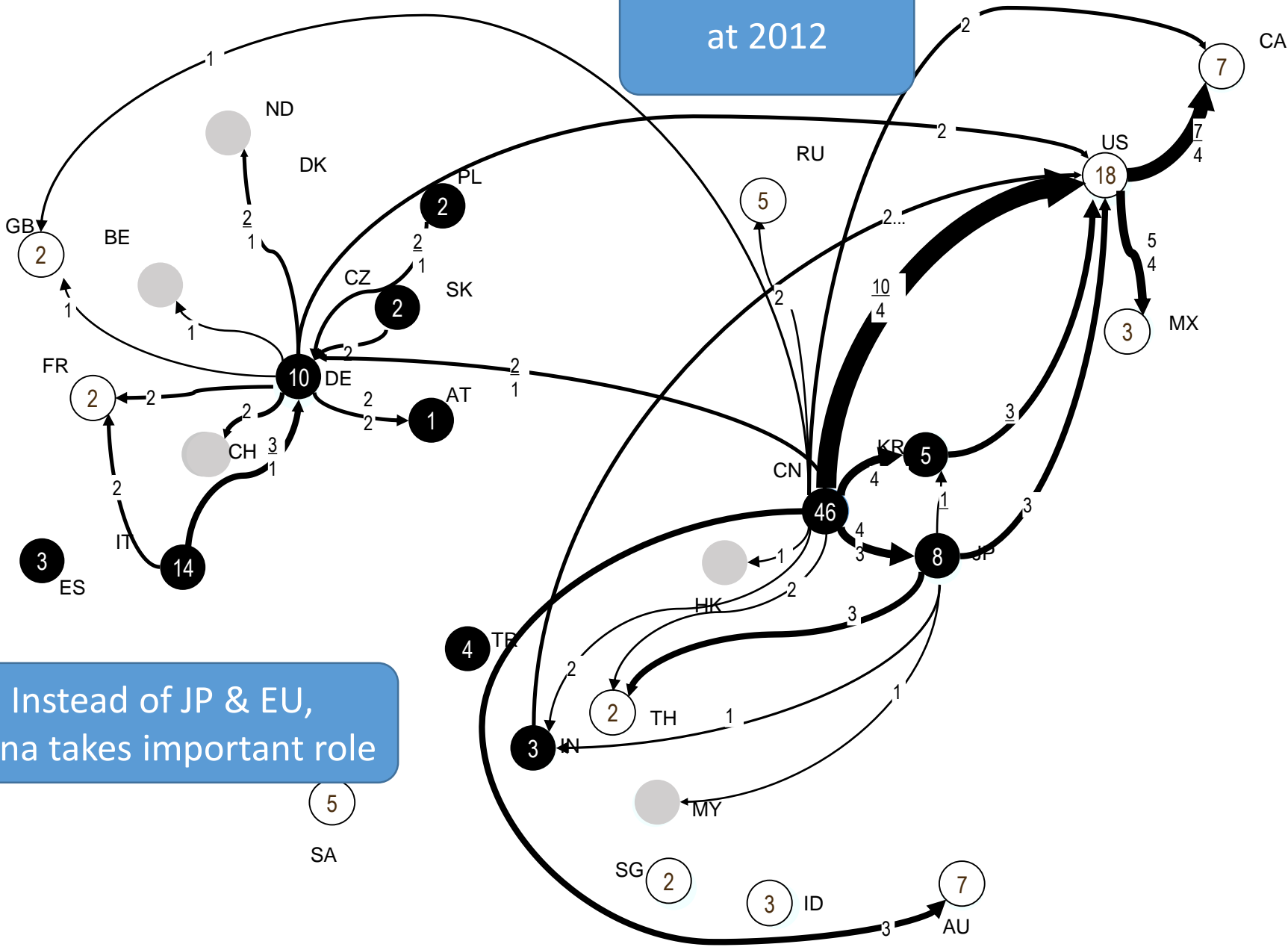
# trade flow of steel at 1992



A typical trilateral structure

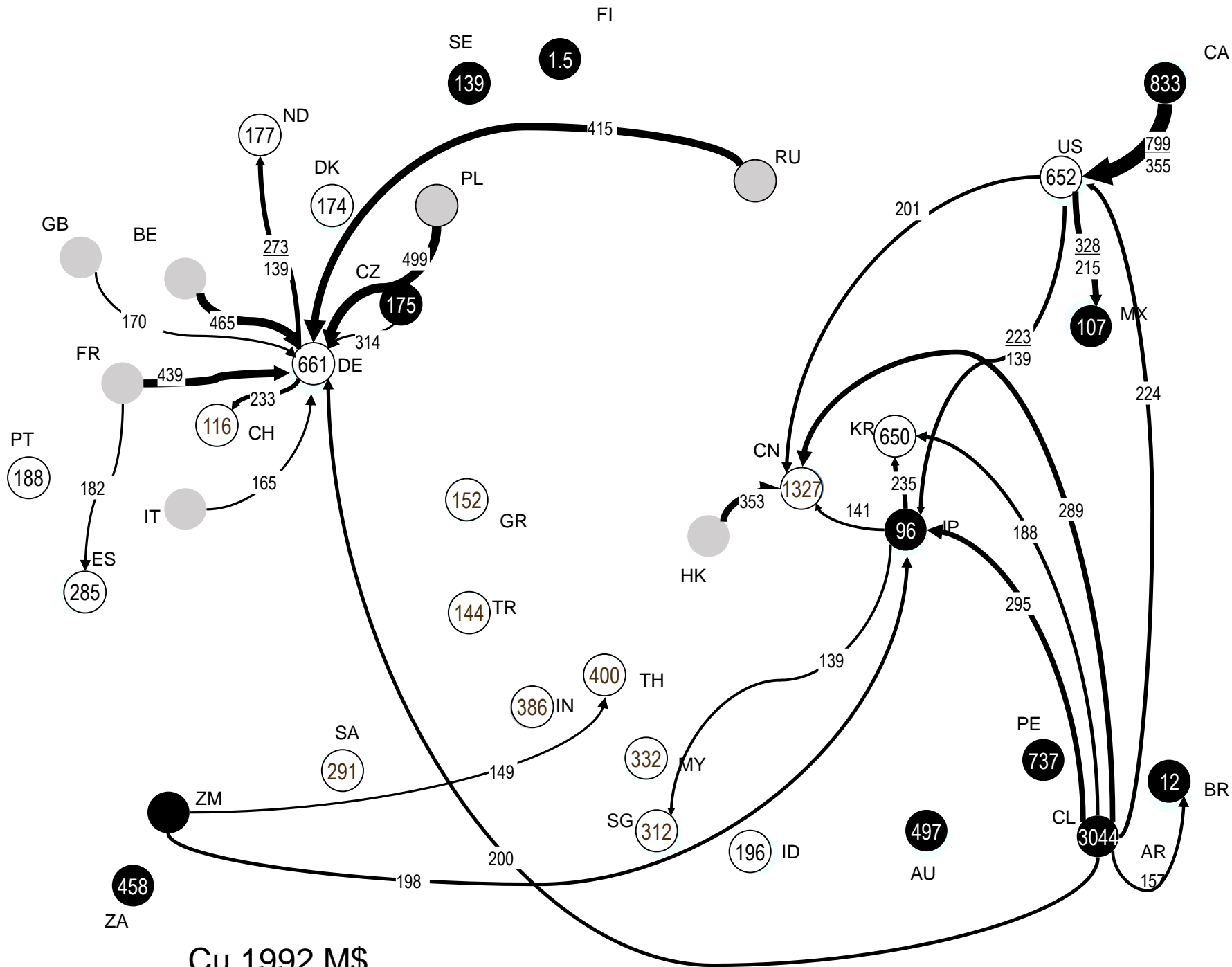
72 Fe 1992 M\$

at 2012



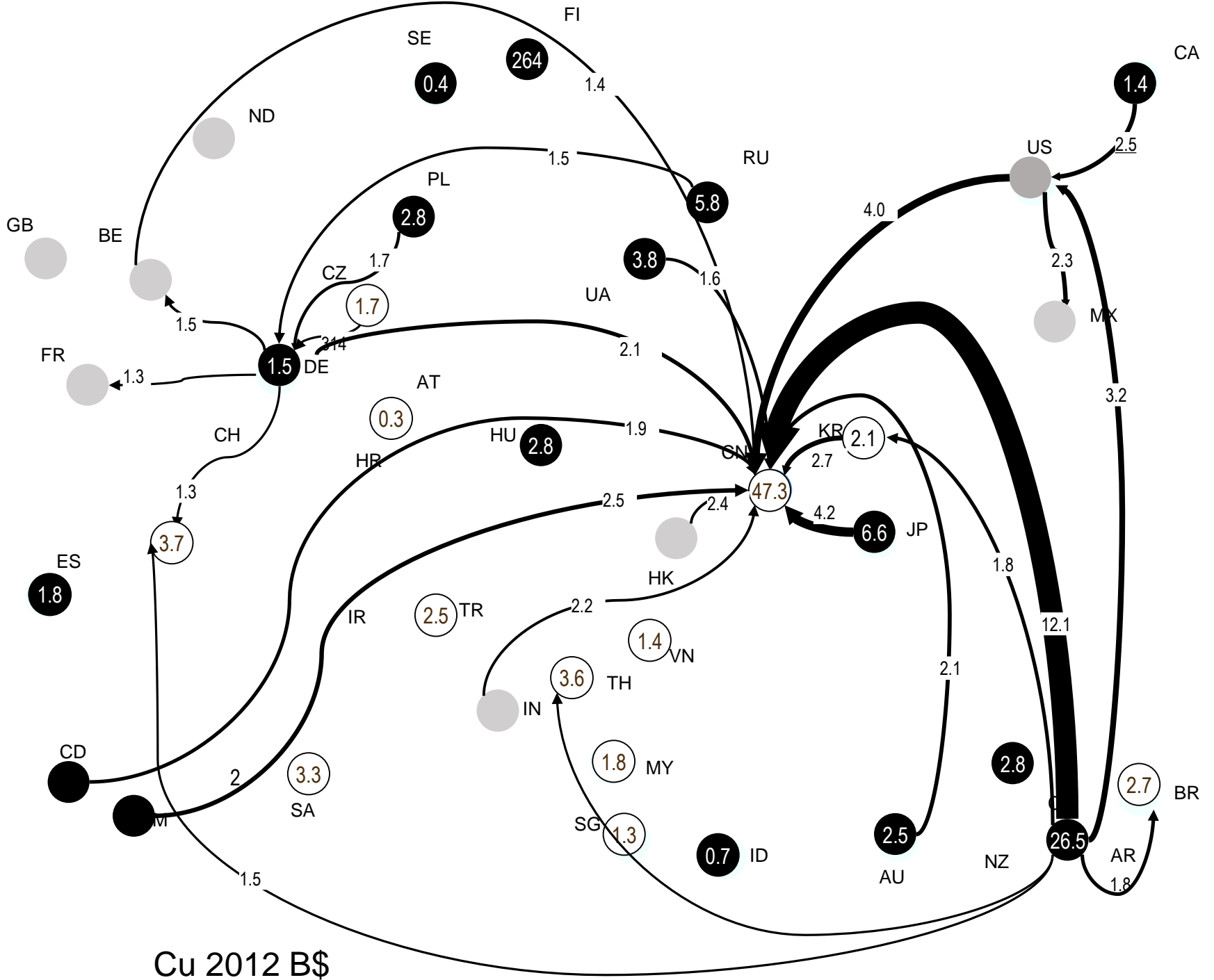
Instead of JP & EU,  
China takes important role

72 Fe 2012 B\$

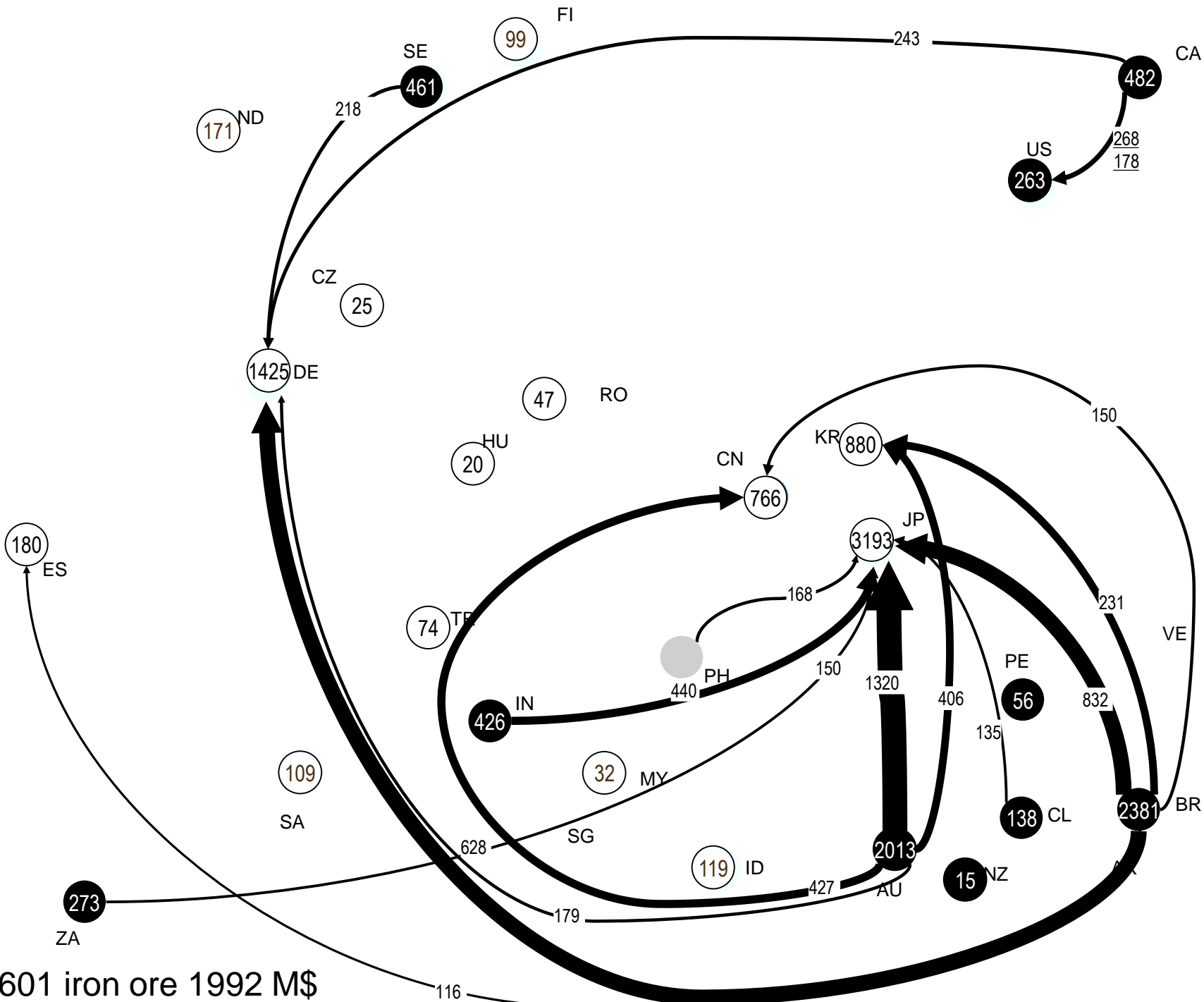


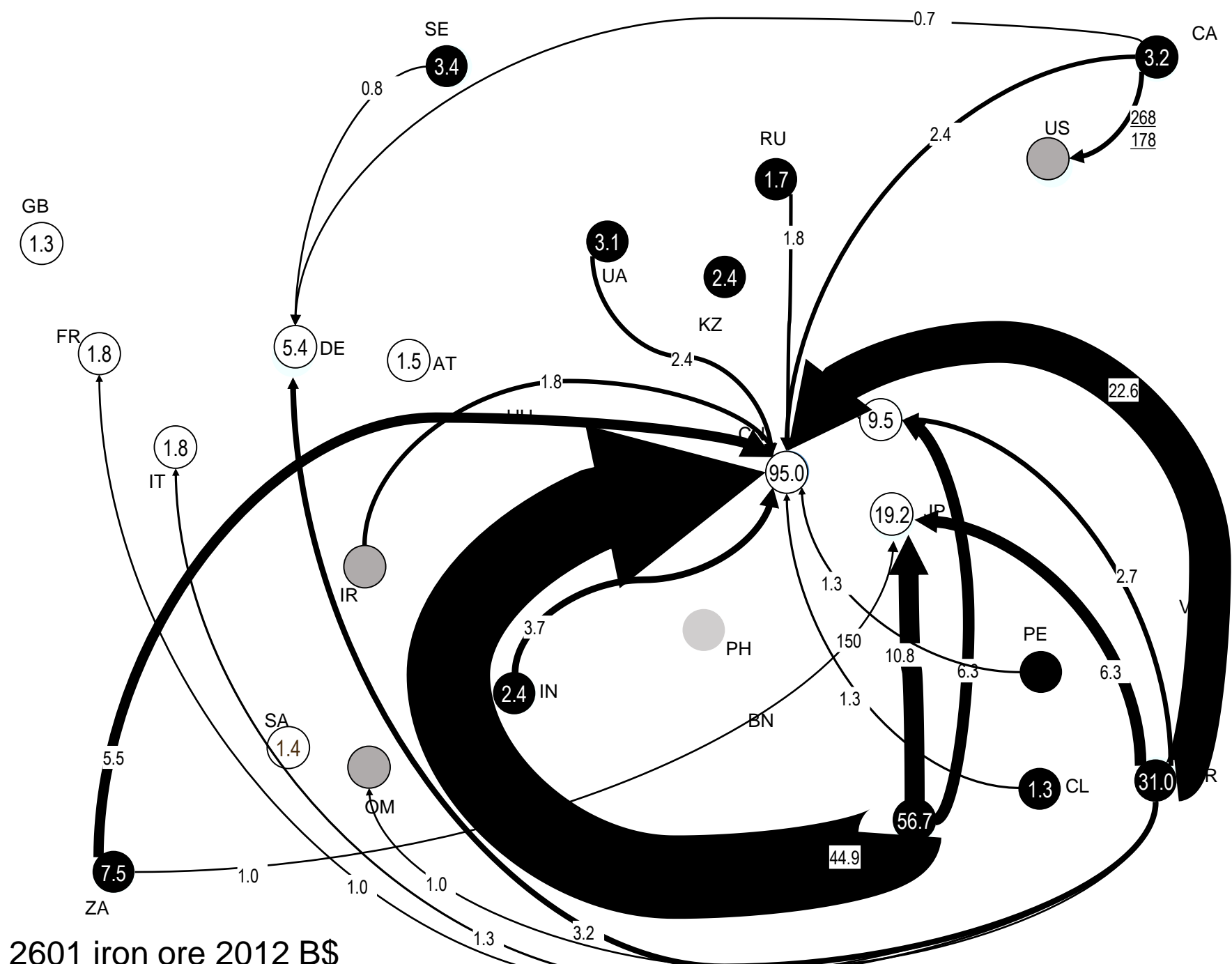
Cu 1992 M\$





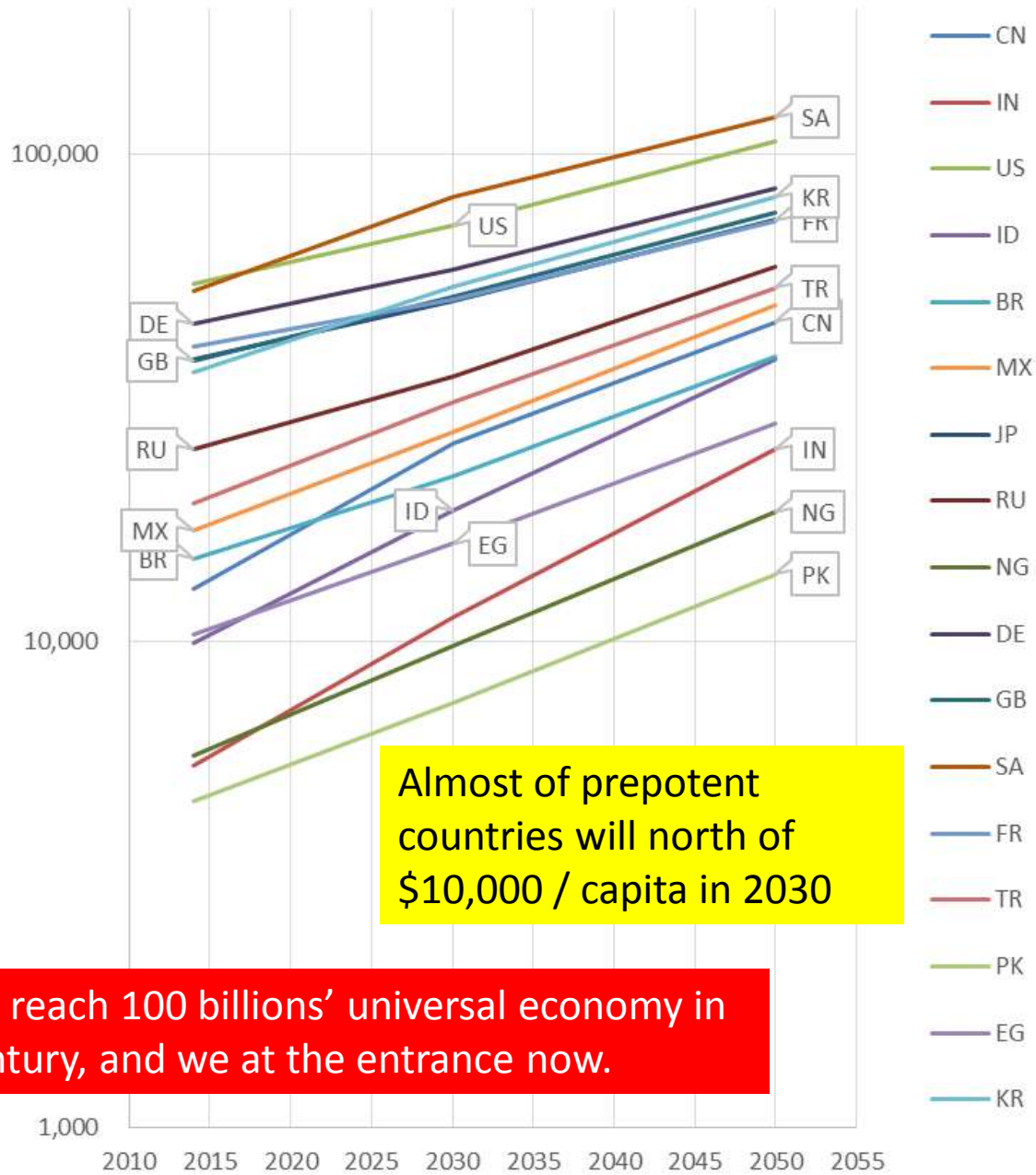
2601 iron ore 1992 M\$







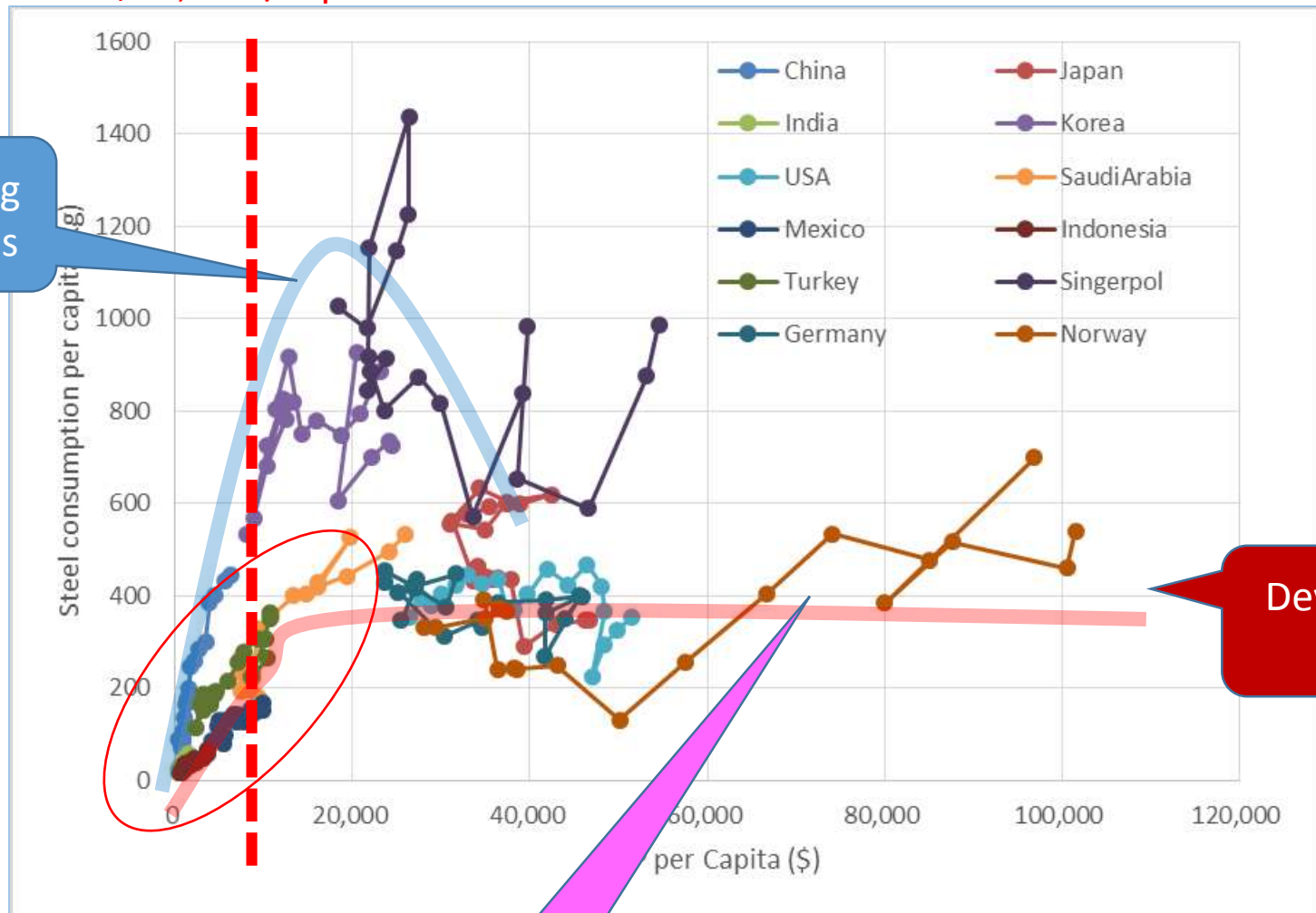
# forecasted GDP per person (PPP base)



Almost of prepotent countries will north of \$10,000 / capita in 2030

We will reach 100 billions' universal economy in this century, and we at the entrance now.

\$10,000 /capita

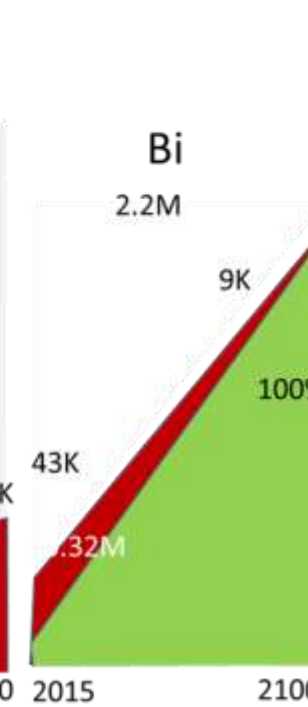
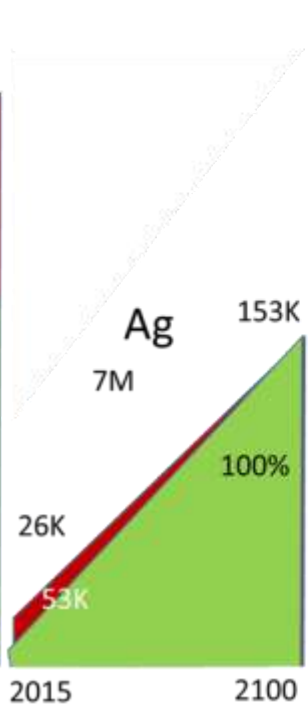
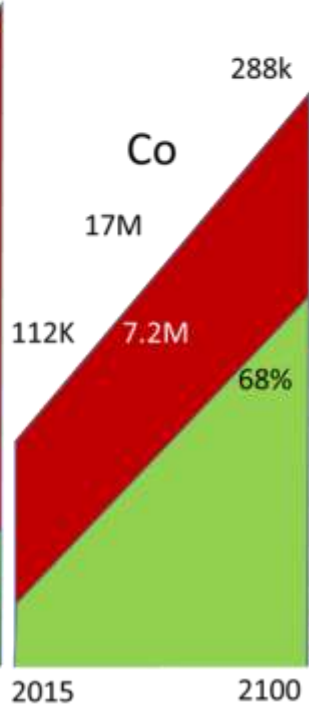
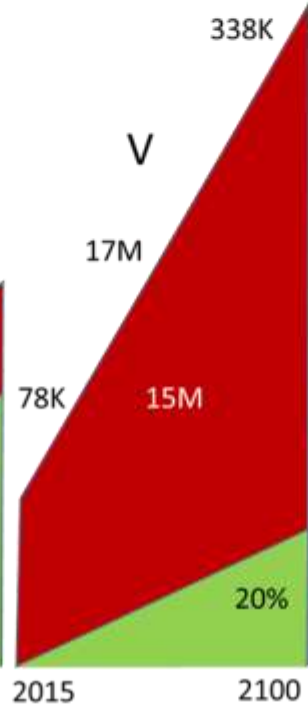
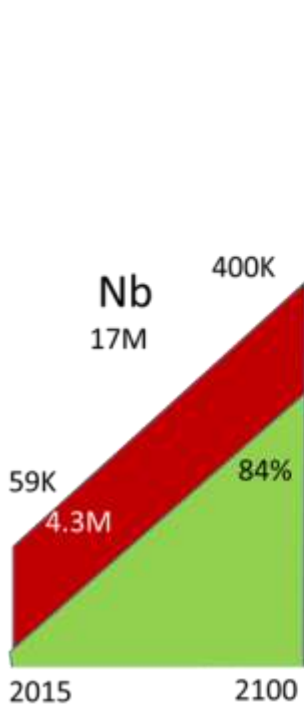
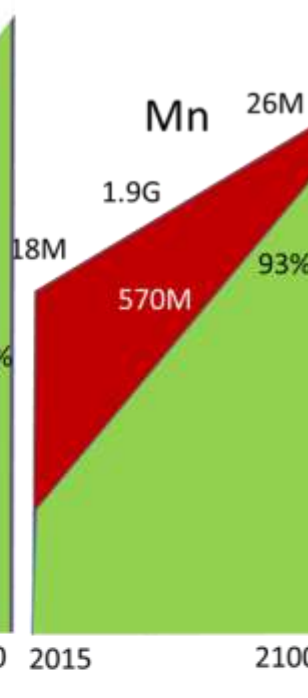
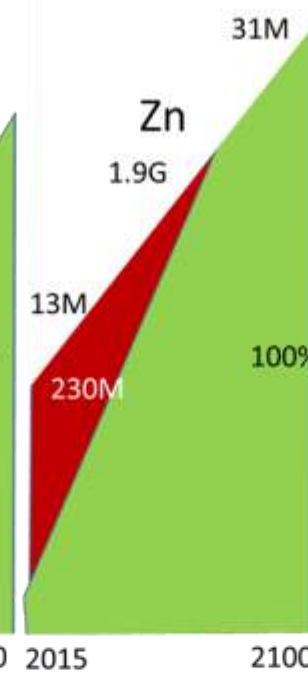
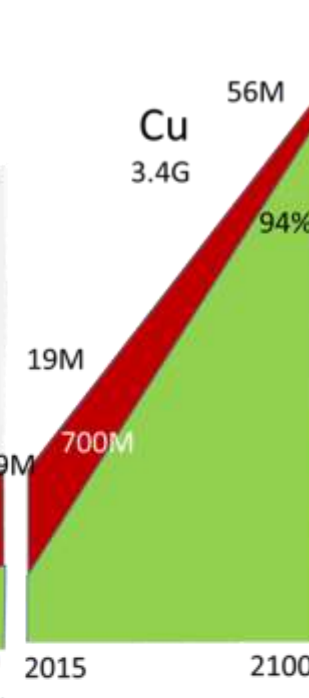
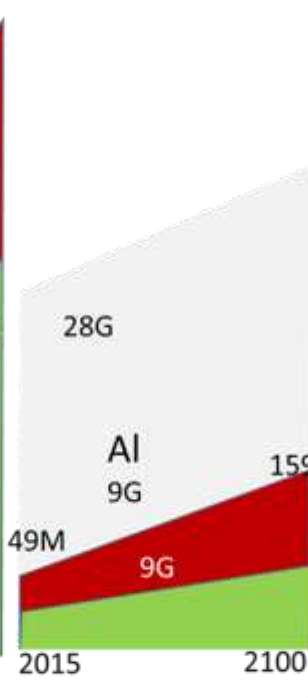
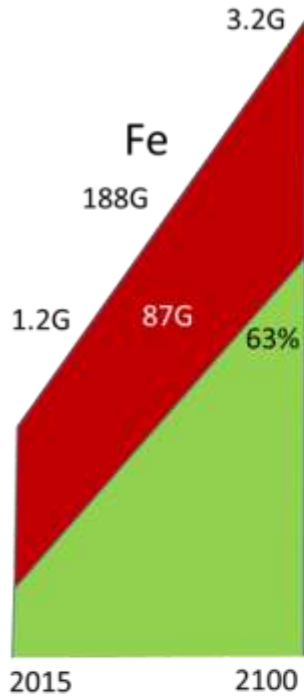


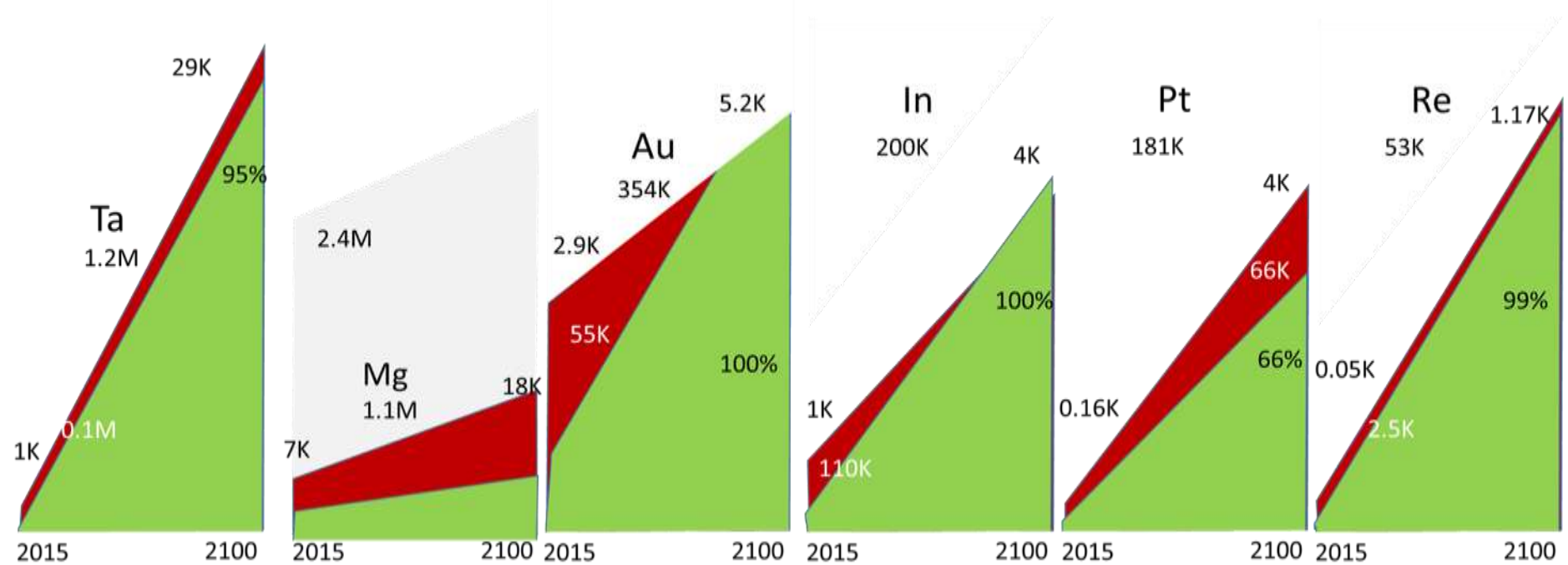
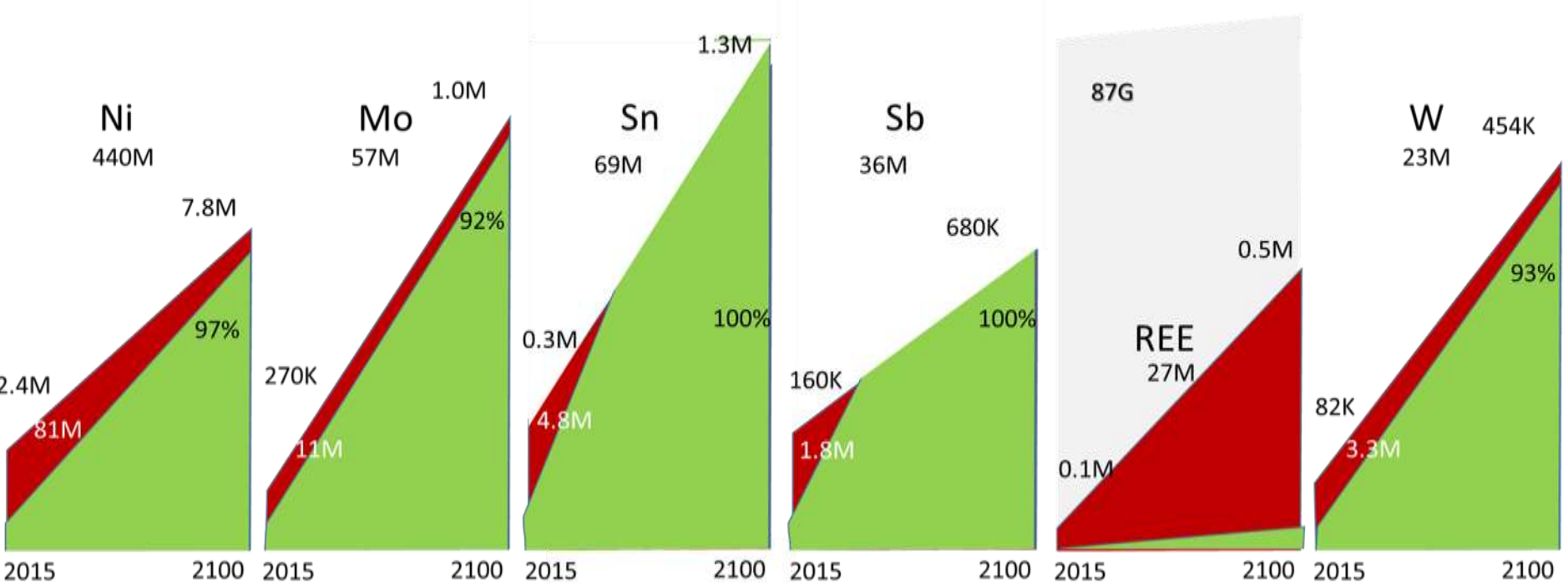
Exporting countries

Developed level

Consuming countries

Fig.8 Fe consumption / capita v.s. GDP/ capita of several countries from 1994 to 2014







# SCIENCE HAS WON AGAINST ECONOMY

- JAPANESE GENSO SENRYAKU  
(PROJECT OF STRATEGIC ADVANCED MATERIALS)  
FOR RARE EARTH AND CRITICAL METALS-

Kohmei HALADA

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National Institute for Materials Science

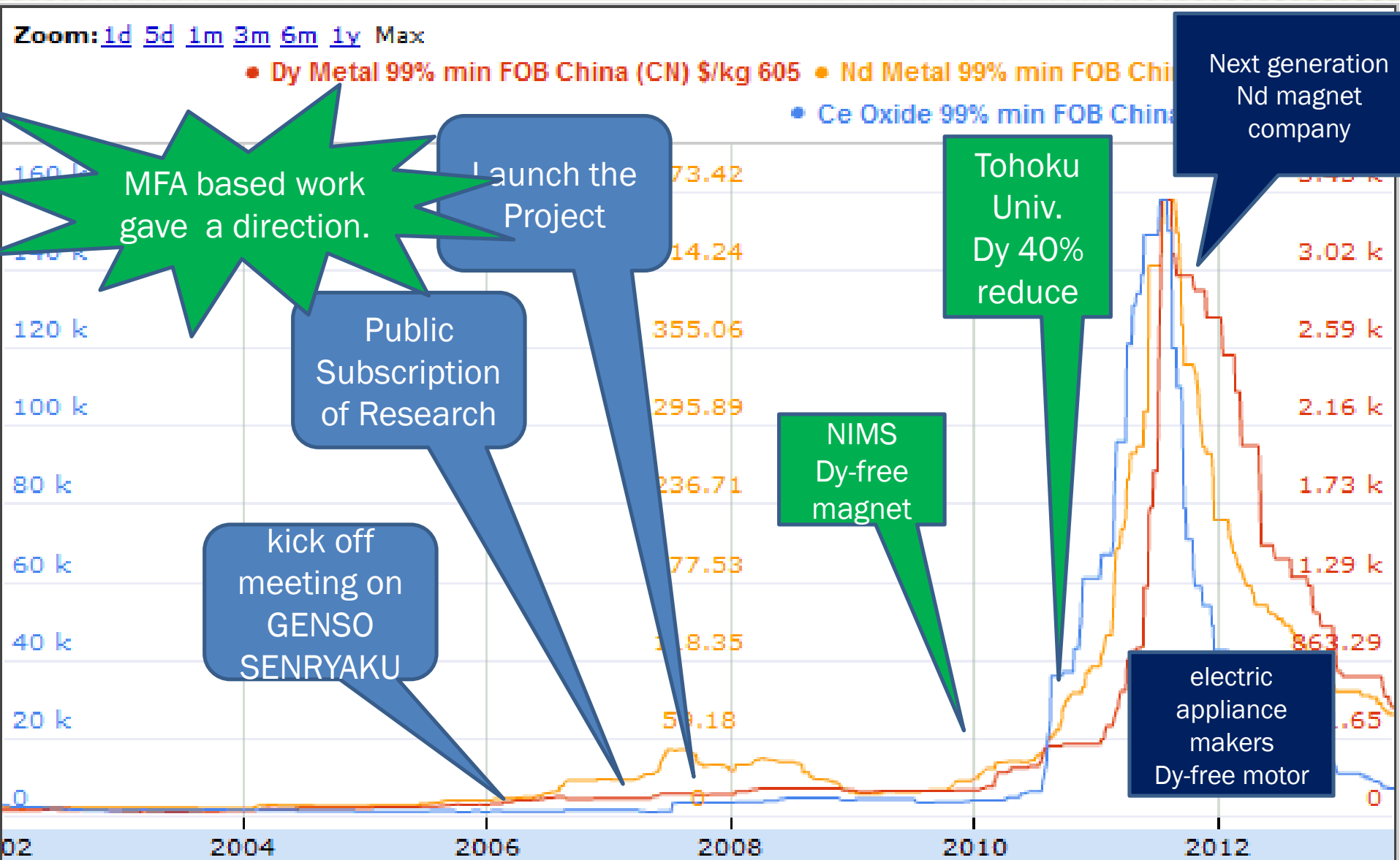
President of Inst. Japan LCA

President of Ecomaterilas Forum

Japan government launch a project named GENSO SENRYAKU

efficient use  
alternatives  
recycling

S&T project for advanced strategic elements

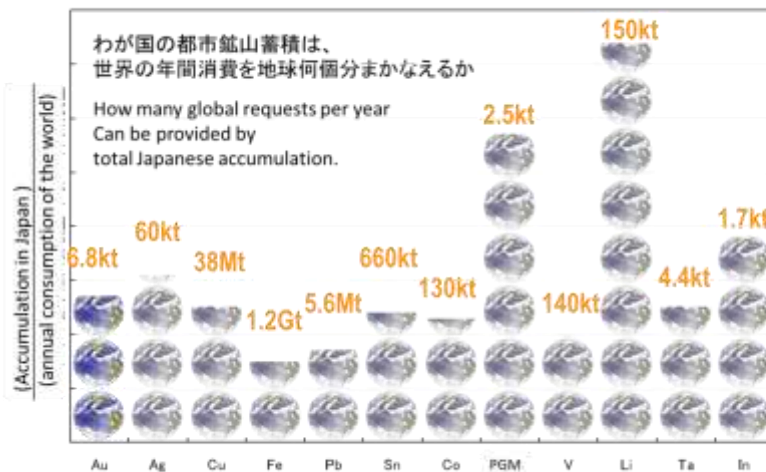


- MFA: tracing tool of the flow in life cycle of material in the society.

Applied for

- Prediction of future consumption
  - Why we should do.
- Estimation of stocked material
  - What we can do.

"Urban mining" had been revived by the work of estimation of domestic accumulation.



Total accumulation in Japan compared with annual consumption in the world

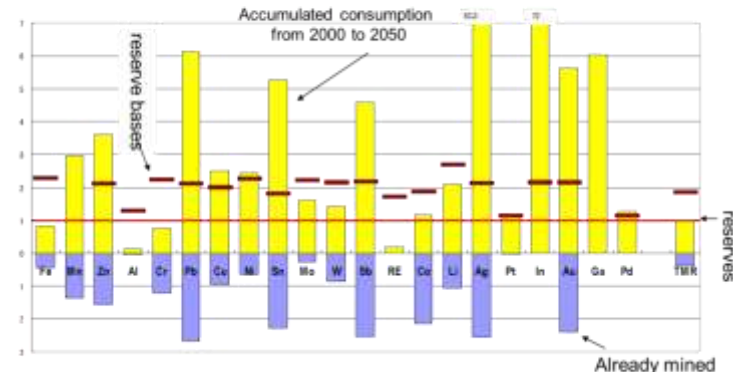
K.Halada et al.: Material Transactions, Vol.49(2008), (in Japanese)

Several times amount of resources will be required by 2050.

It will be close to the amount of reserve by 2050: Fe, Mo, W, Co, Pt, Pd

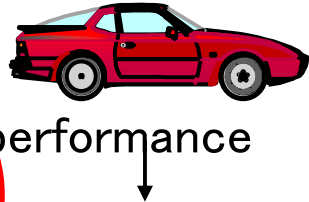
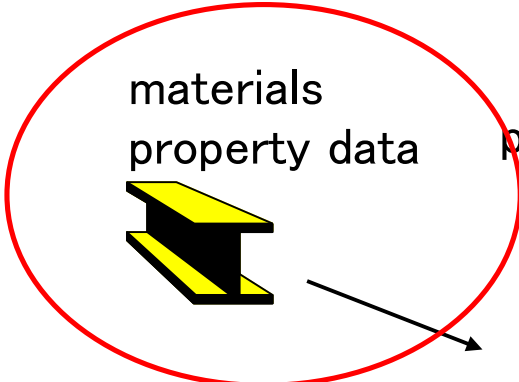
It will require several times amount of reserve by 2050: Ni, Mn, Li, In, Ga

It will run over the amount of reserve base by 2050: Cu, Pb, Zn, Au, Ag, Sn



K.Halada et al.: Forecasting of the Consumption of Metals up to 2050, Material Transactions, Vol.49(2008), No.3,402-410 (Japanese Ver, 2007)





scenario of usage

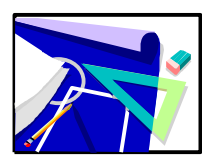
scenario of disposal



LCI data of materials

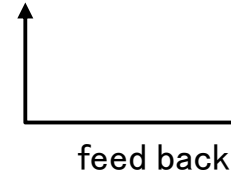


Life cycle simulation



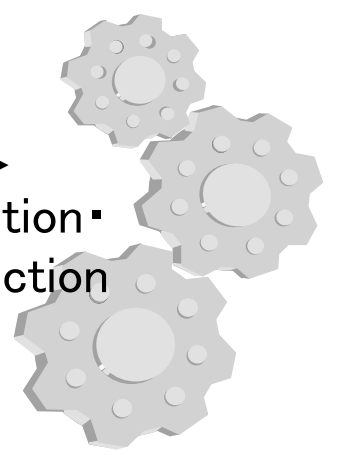
DfE(Design for Environment)elements

- easy to disassemble
- easy to reuse
- easy to discriminate
- etc.

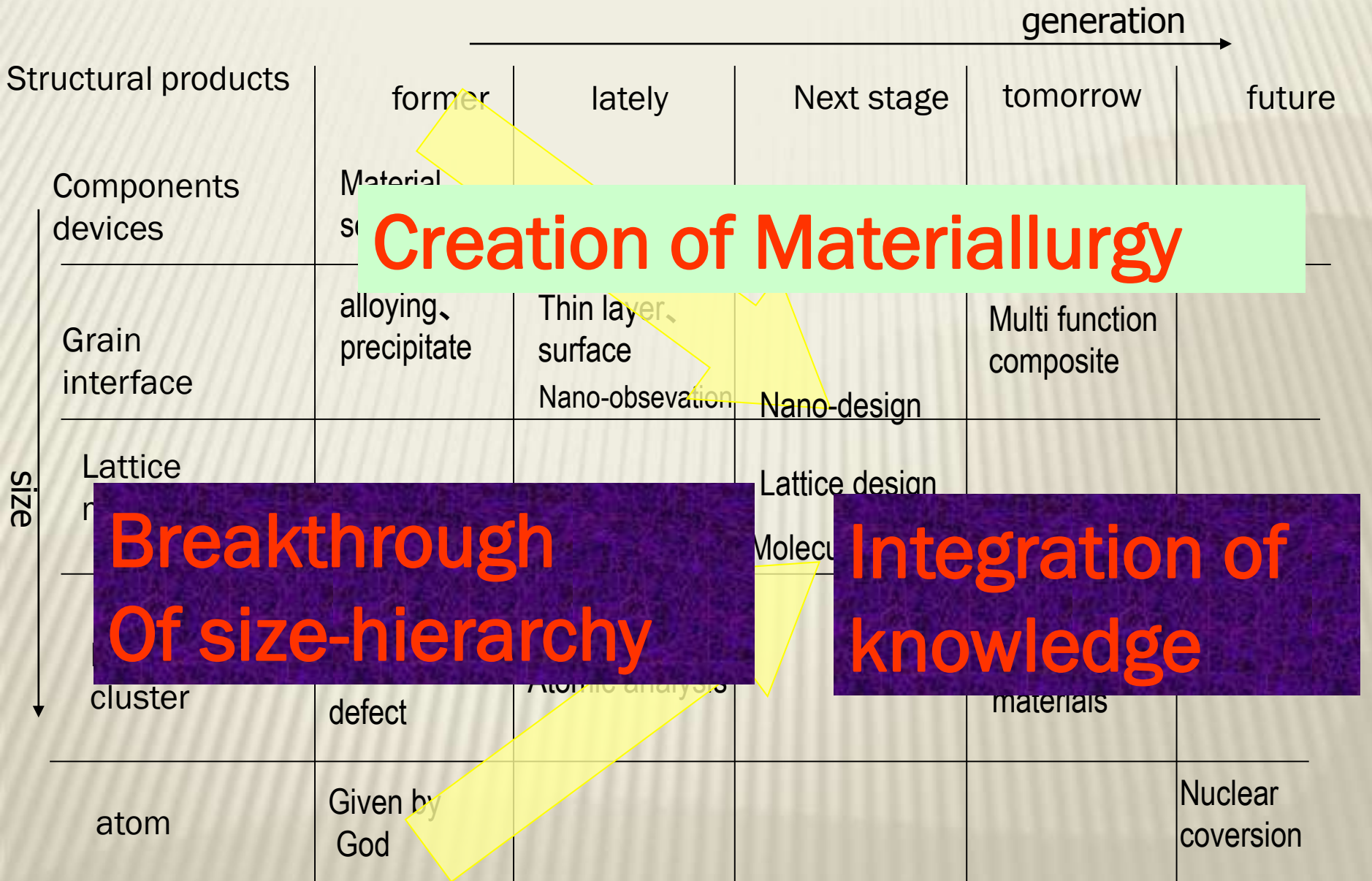


Linkage of LCA to LCE

aquisition - production



Now we are at the meeting point of nano-size and macro-size



**Creation of Materiallurgy**

**Breakthrough  
Of size-hierarchy**

**Integration of  
knowledge**

**Nano-alchemy: converging technology** of physics, chemistry, metallurgy

# Elements Strategy Initiative

## Inter-Disciplinary and Cross-Sectoral Collaboration

### [Enforcement of Scientific Fundamentals and Integration of Advanced Knowledge and Technologies]



### [Inter-Ministry network for Permanent Magnet Development]



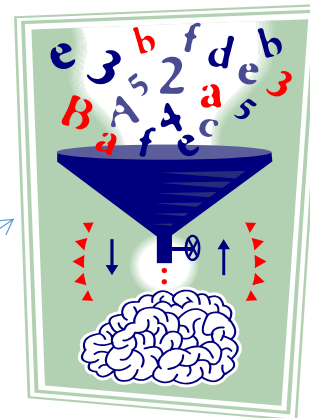


reader

ACCESS:

documents+  
parameter

big data



Free dimension publish



multifunction, large, complex data are directly referred.

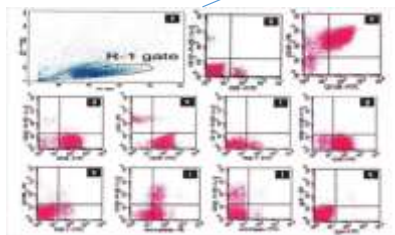
PUBLISH:

documents+  
parameter

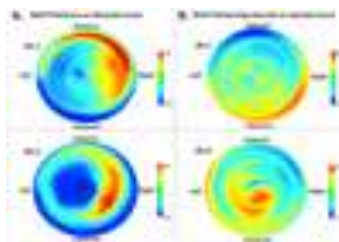


author

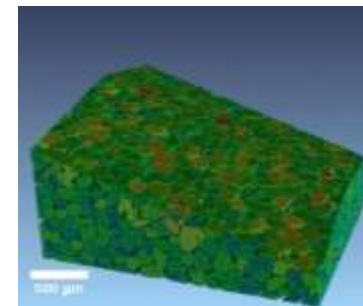
common procedure ( ex.HDF5)



multi parameter data



4D data

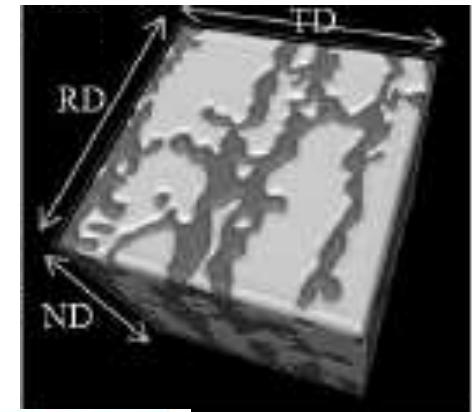
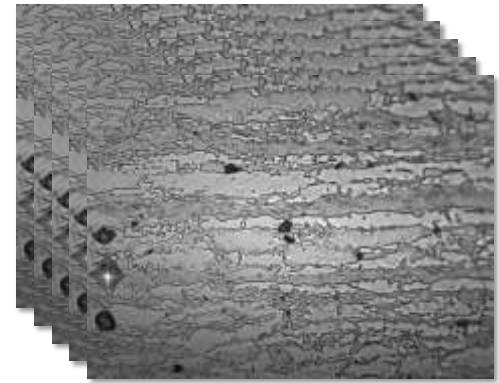
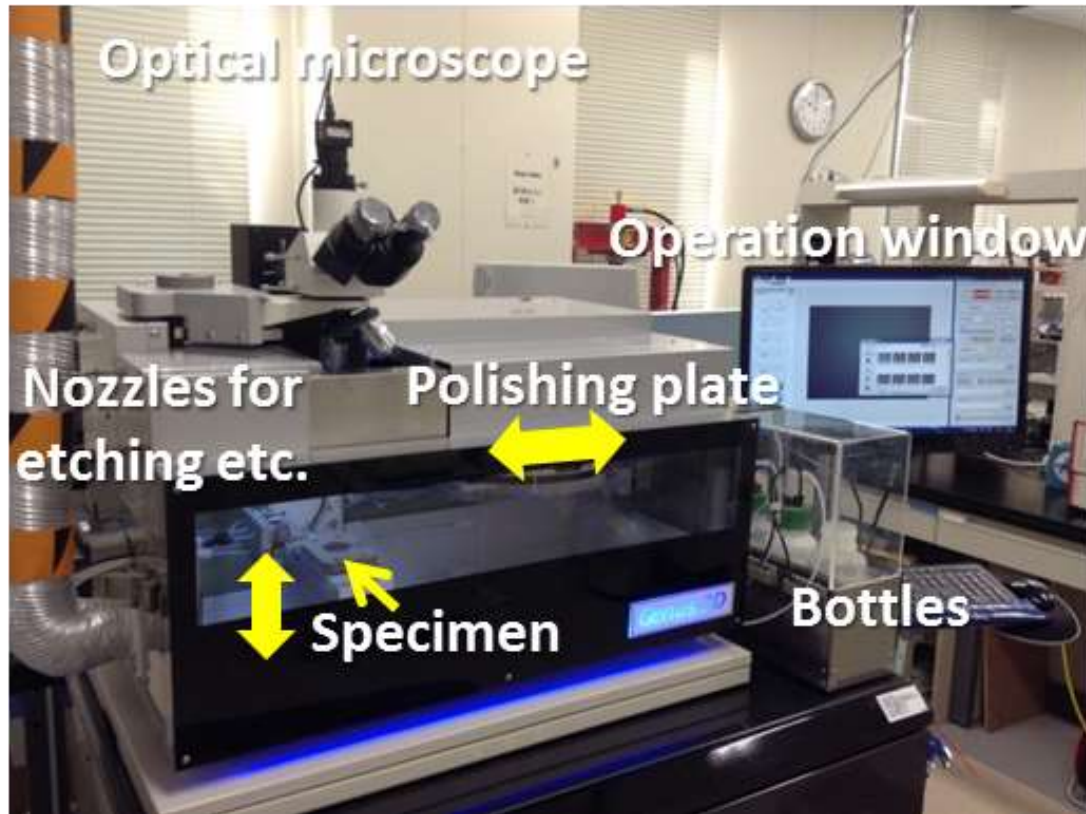


3D data



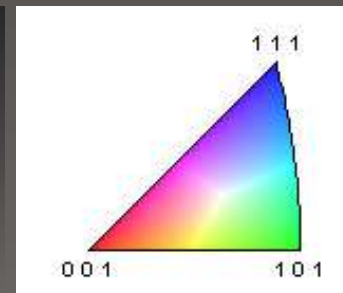
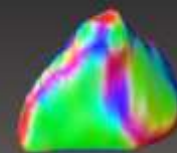
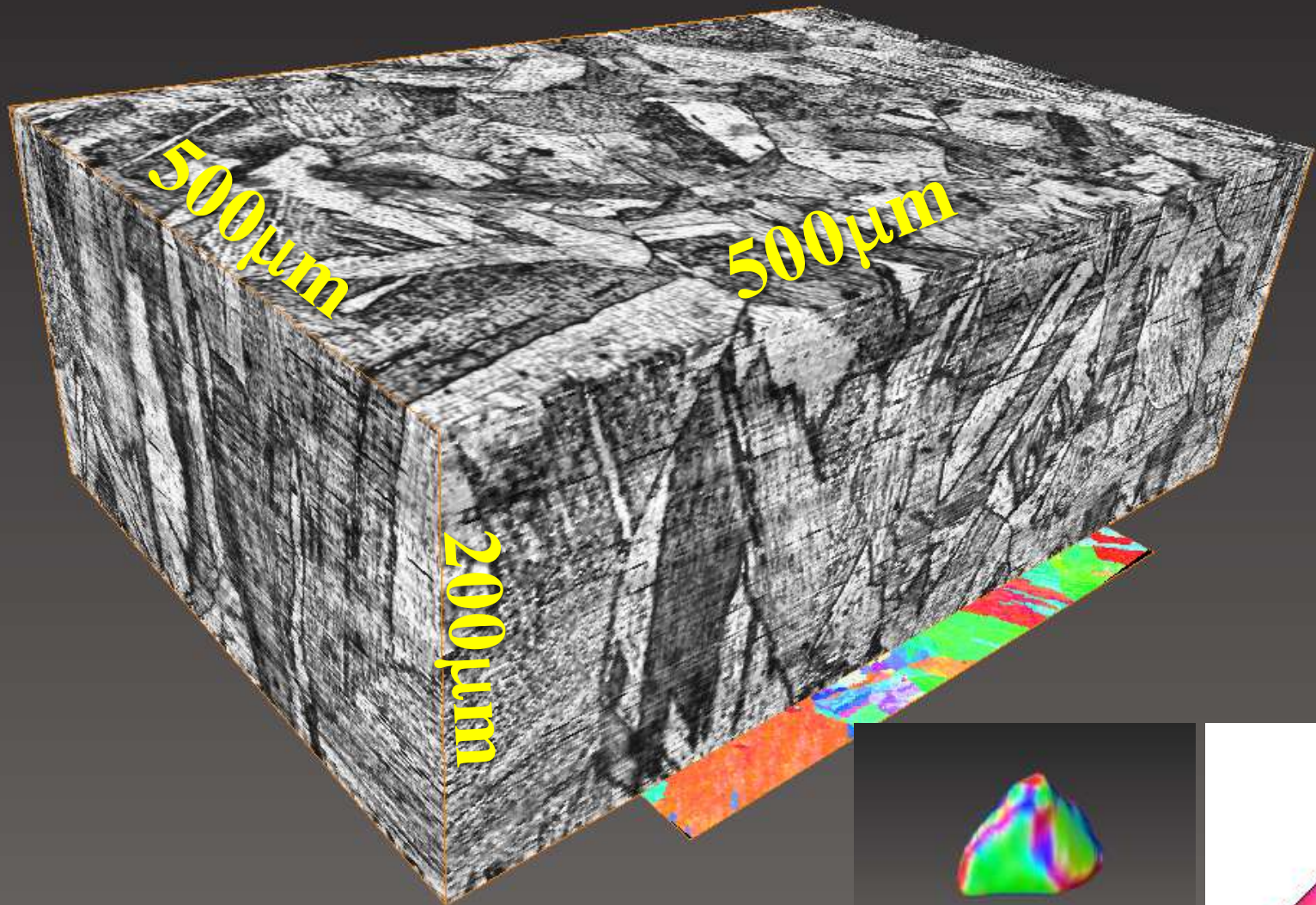
# Genus 3D

Fully automated serial sectioning 3D microscope



Prof. Adachi

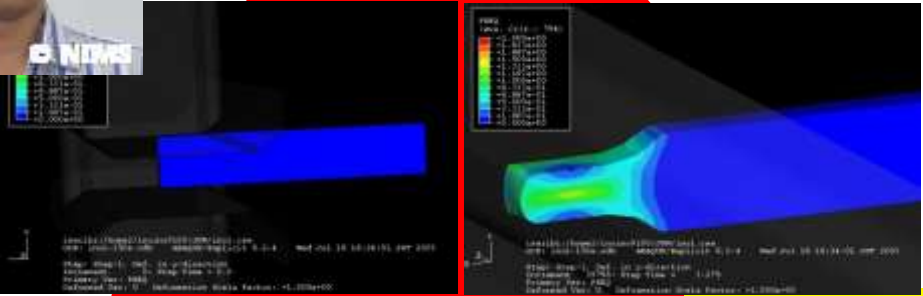
# Lath martensite



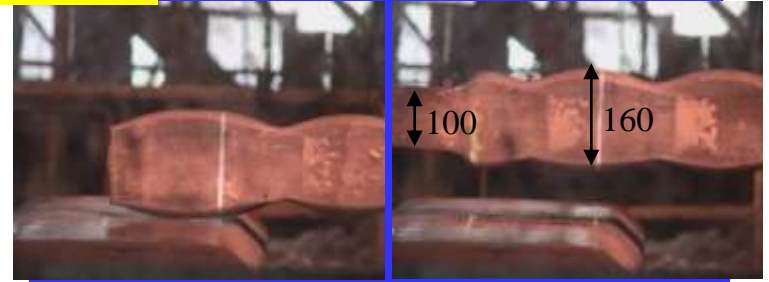
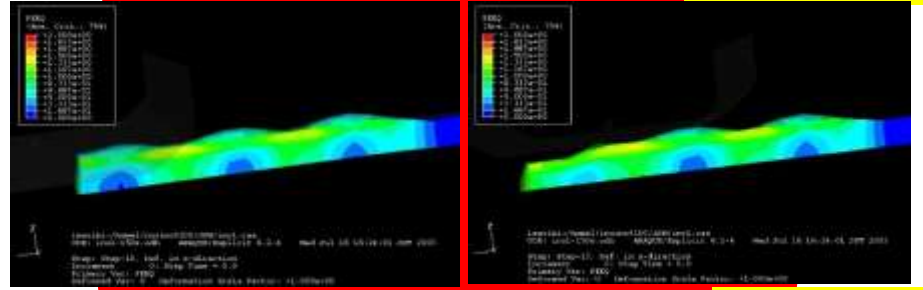
# Numerical approach

# Experimental approach

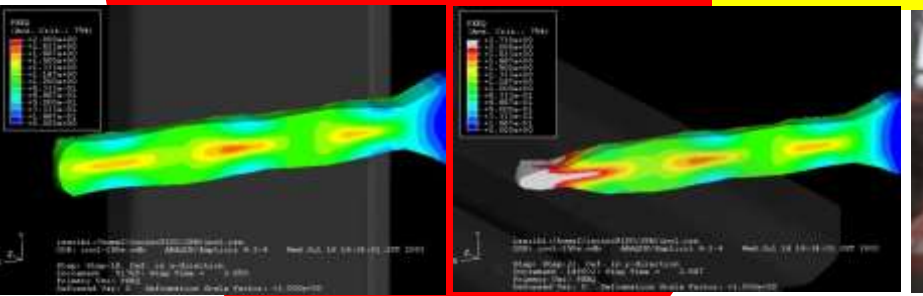
1工程目 (150→75mm)



2工程目 (160→100mm)

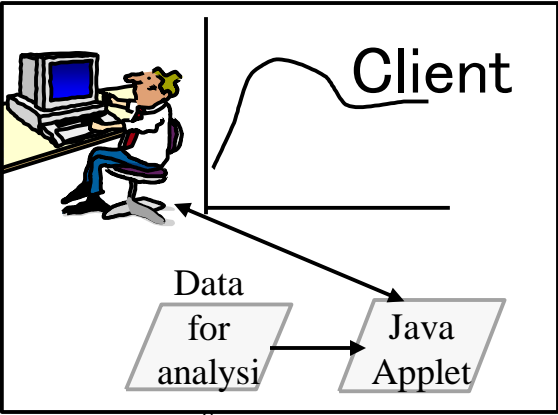


3工程目 (102→34mm)



仮想実験

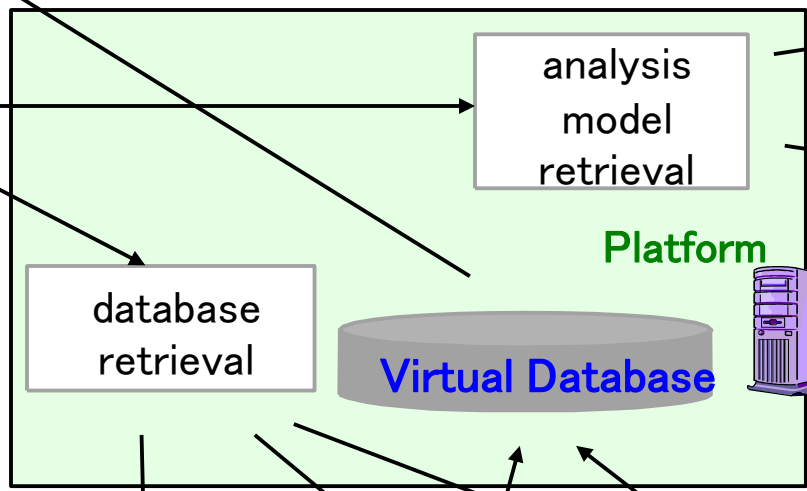
実証実験



**Virtual database**

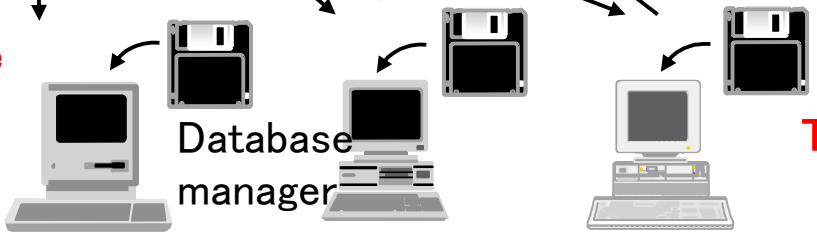
**With generic format**

**Written with common Markup-Language**

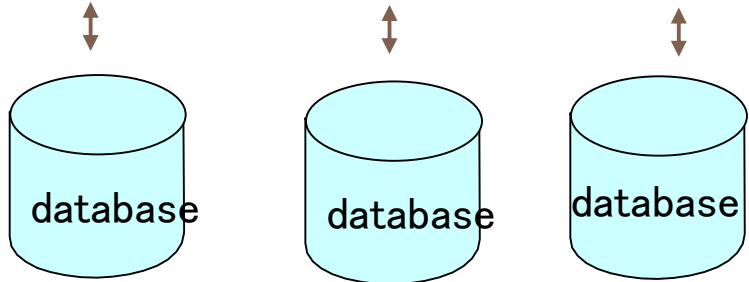


Data analysis model

**Template**



**Template**



Every database has its own **logic**, **metadata**, and **structure** depending on their aim and scope.

Users are required to **learn the structure of each database** to retrieve and obtain data.

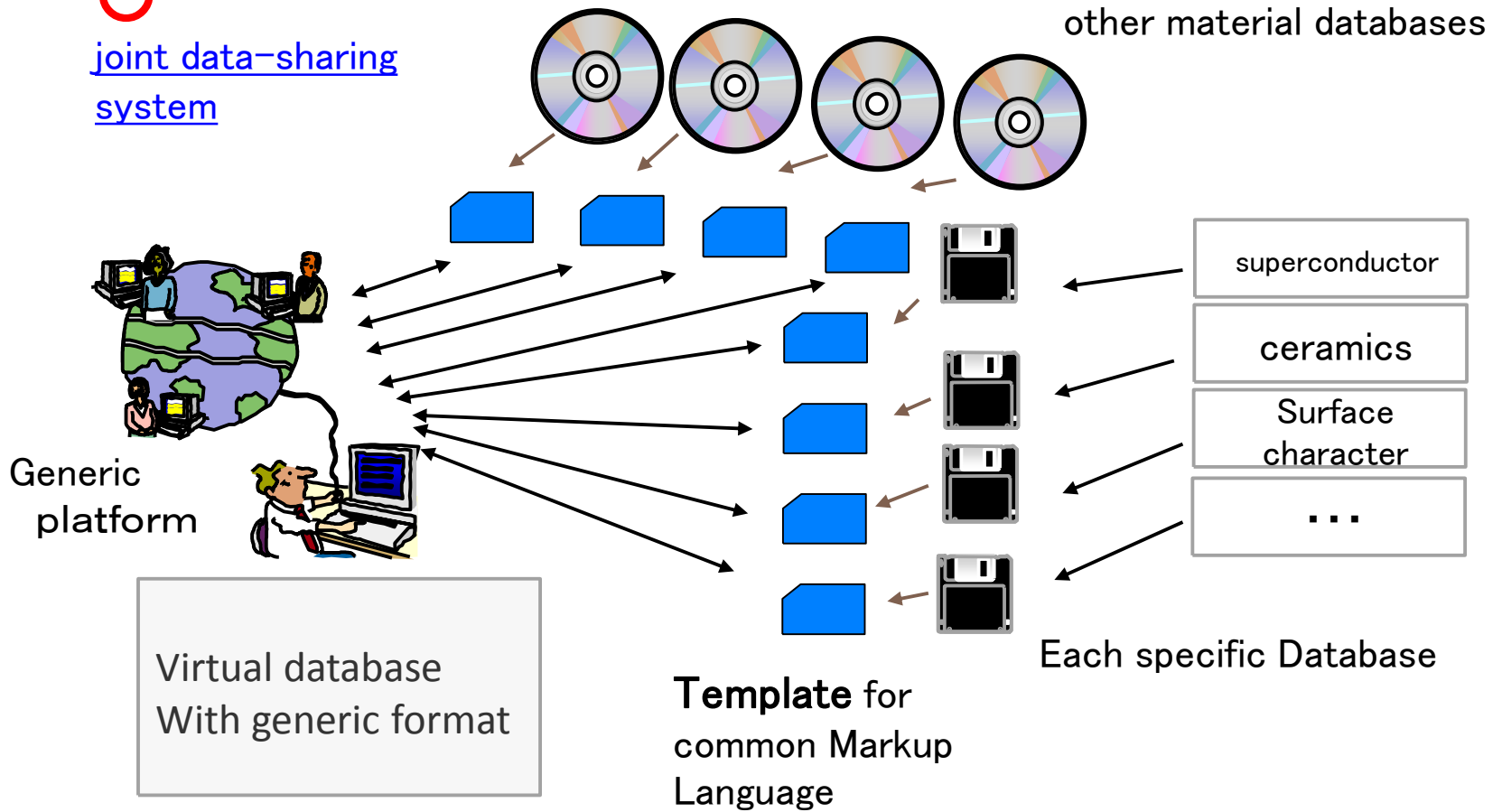
If **man feels difficult** to read and exchange them among different databases,  
then **machine cannot exchange** them automatically.

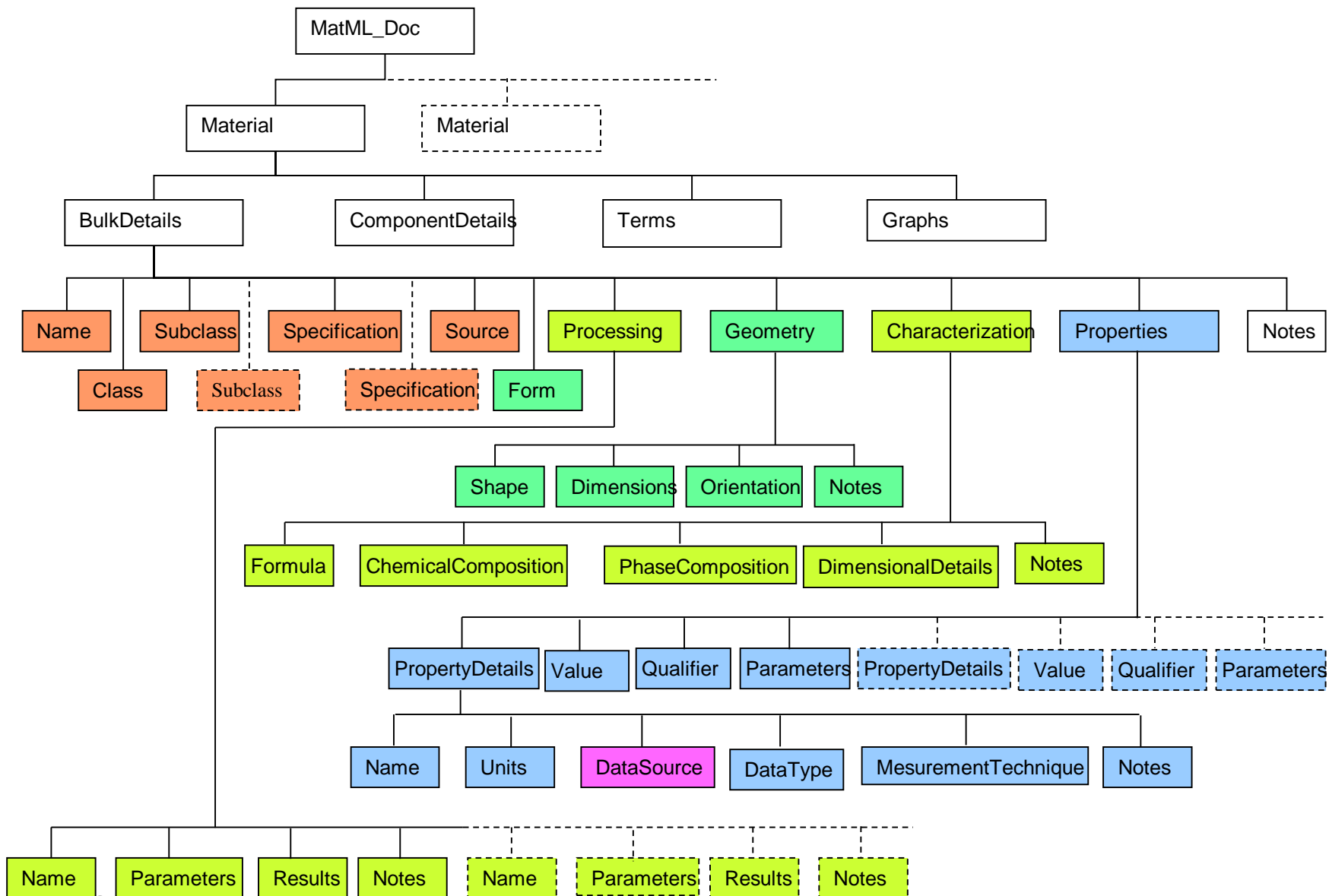
The approaches of **common database** and **common format** have failed because;

- a) The **structure depends on the logic** which is specifically reflected by the object and the aim of database.
- b) The **metadata cannot determined universally**, because terminological interpretation has discrepancies among the specific fields and languages.



joint data-sharing system





```

<?xml version="1.0"?>
<!DOCTYPE Data SYSTEM "my-creep.dtd">
<Data>
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  </Specimen_Information>
  <Test_Results>
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      <Creep_Rupture_Data>
        <Time_Strain_Data>
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          <Time unit="h">648.0</Time> <Strain unit="percent">2.045</Strain>
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      </Creep_Rupture_Data>
    </Result_of_Creep_Rupture>
  </Test_Results>
  <Test_Validation/>
</Material_Property>
</Data>

```



## problem of “A of B” and “A of C”

two different cases exists

### common item

“A” of “A of B” and “A” of “A of C” are same “A”

### inherited item

“A” of “A of B” and “A” of “A of C” are different “A”

some solution

### common item

→ name space

### inherited item

→ modified description of TAG such as <B\_A>

→ for the classification, the expert knowledge of materials engineer is necessary.

## Distinction of the Relation among the elements

How to weigh the importance of the elements

In a creep data

<Grain\_Size>**2.5**</Grain\_Size>

<Hardness>**88**</Hardness>

<Time\_to\_Rupture>**24651.5**</Time\_to\_Rupture>

How to present the relation among the elements

In a creep data

<Rupture\_Data>

<Time\_to\_Rupture>**24651.5**</Time\_to\_Rupture>

<Elongation>**41.3**</Elongation>

<Reduction\_of\_Area>**85.1**</Reduction\_of\_Area>

</Rupture\_Data>

for Large data

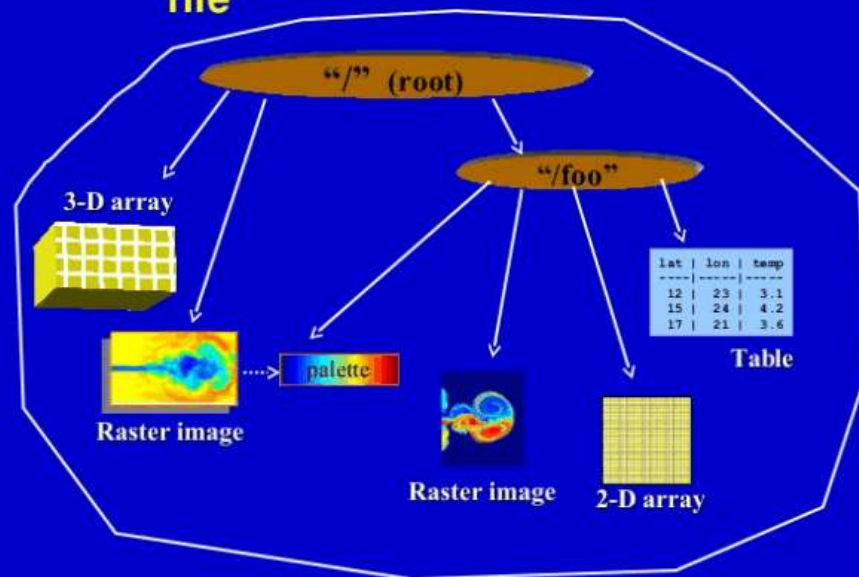
Clip slide

# Introduction to HDF5 Data Model, Programming Model and Library APIs

HDF and HDF-EOS Workshop VIII  
October 26, 2004

1

## Example HDF5 file



## Dataset Components

Clip slide

**Metadata**

**Dataspace**

Rank	Dimensions
3	Dim_1 = 4 Dim_2 = 5 Dim_3 = 7

**Datatype**

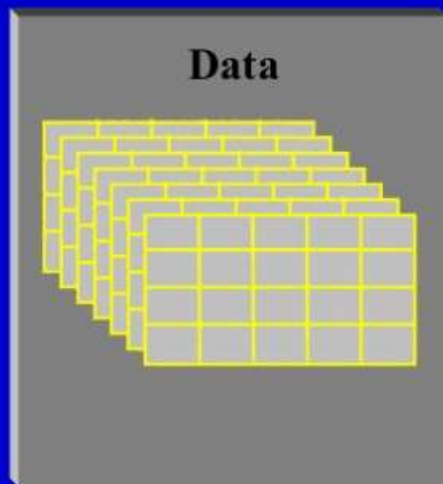
IEEE 32-bit float

**Attributes**

Time = 32.4
Pressure = 987
Temp = 56

**Storage info**

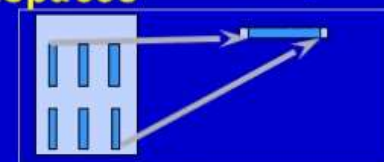
Chunked  
Compressed



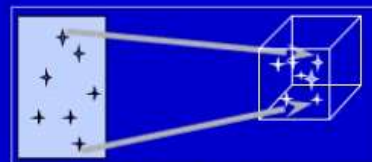
## Sample Mappings between File Dataspaces and Memory Dataspaces



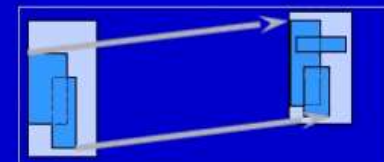
(a) Hyperslab from a 2D array to the corner of a smaller 2D array



(b) Regular series of blocks from a 2D array to a contiguous sequence at a certain offset in a 1D array





(c) A sequence of points from a 2D array to a sequence of points in a 3D array.

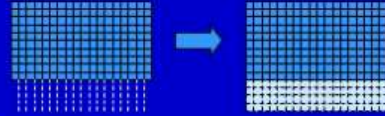


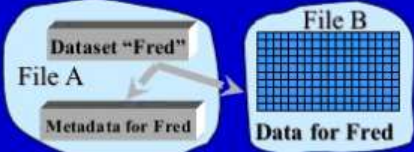
(d) Union of hyperslabs in file to union of hyperslabs in memory.

## Special Storage Options

**chunked**  Better subsetting access time; extendable

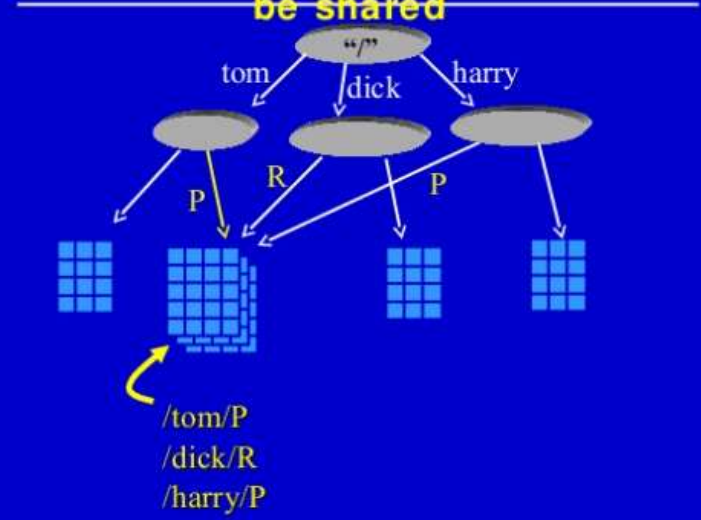
**compressed**  Improves storage efficiency, transmission speed

**extendable**  Arrays can be extended in any direction

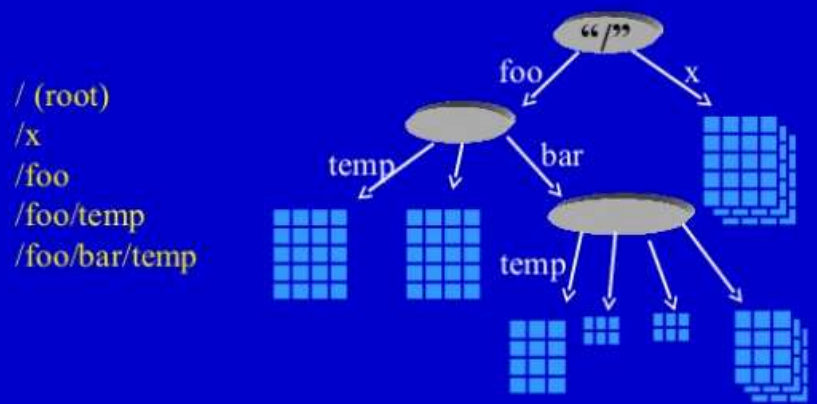
**External file**  Metadata in one file, raw data in another.

## Groups & members of groups can

be shared



## HDF5 objects are identified and located by their pathnames



## Example 2 – Create an empty 4x6 dataset

```

1 hid_t      file_id, dataset_id, dataspace_id;
2 hsize_t    dims[2];
3 herr_t     status;

4 file_id = H5Fcreate ("dset.h5", H5F_ACC_TRUNC,
                    H5P_DEFAULT, H5P_DEFAULT);

5 dims[0] = 4;
6 dims[1] = 6;
7 dataspace_id = H5Screate_simple (2, dims, NULL);
8 dataset_id = H5Dcreate(file_id, "dset", H5T_STD_I32BE,
                    dataspace_id, H5P_DEFAULT);
9 status = H5Dclose (dataset_id);
10 status = H5Sclose (dataspace_id);
11 status = H5Fclose (file_id);
    
```

Create a dataset

Pathname

Datatype

Dataspace

Property list (default)

# Source of bigdata

- Sharing large data which are difficult to obtain
- Daily primary measured and controlled data.
- Failure data  
(Failure is depending on the interpretation but facts. Facts should be accumulated.)
- Interpretation knowledge itself

# Interpretation knowledge and ontology

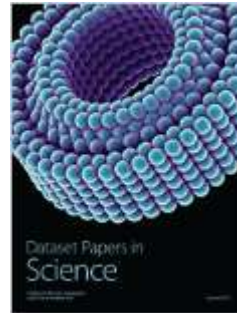
- Database managers has been discussing ontology (relation of terminology).
- But ontology is depending on the individual discipline as the structure of the logic.
- As informatics is the communication beyond discipline, interpretation knowledge such as relation of terminology is extracted from bigdata of interpretation.

# Data journal

- Digitalized journal which can refer large size data or visualize movies.
- Why we have to shrink data into 2-dimensional expression and limited number? Traceability and transparency is already approaching the limit.
- Data journal has possibility to prepare bigdata platform by its free description of data.

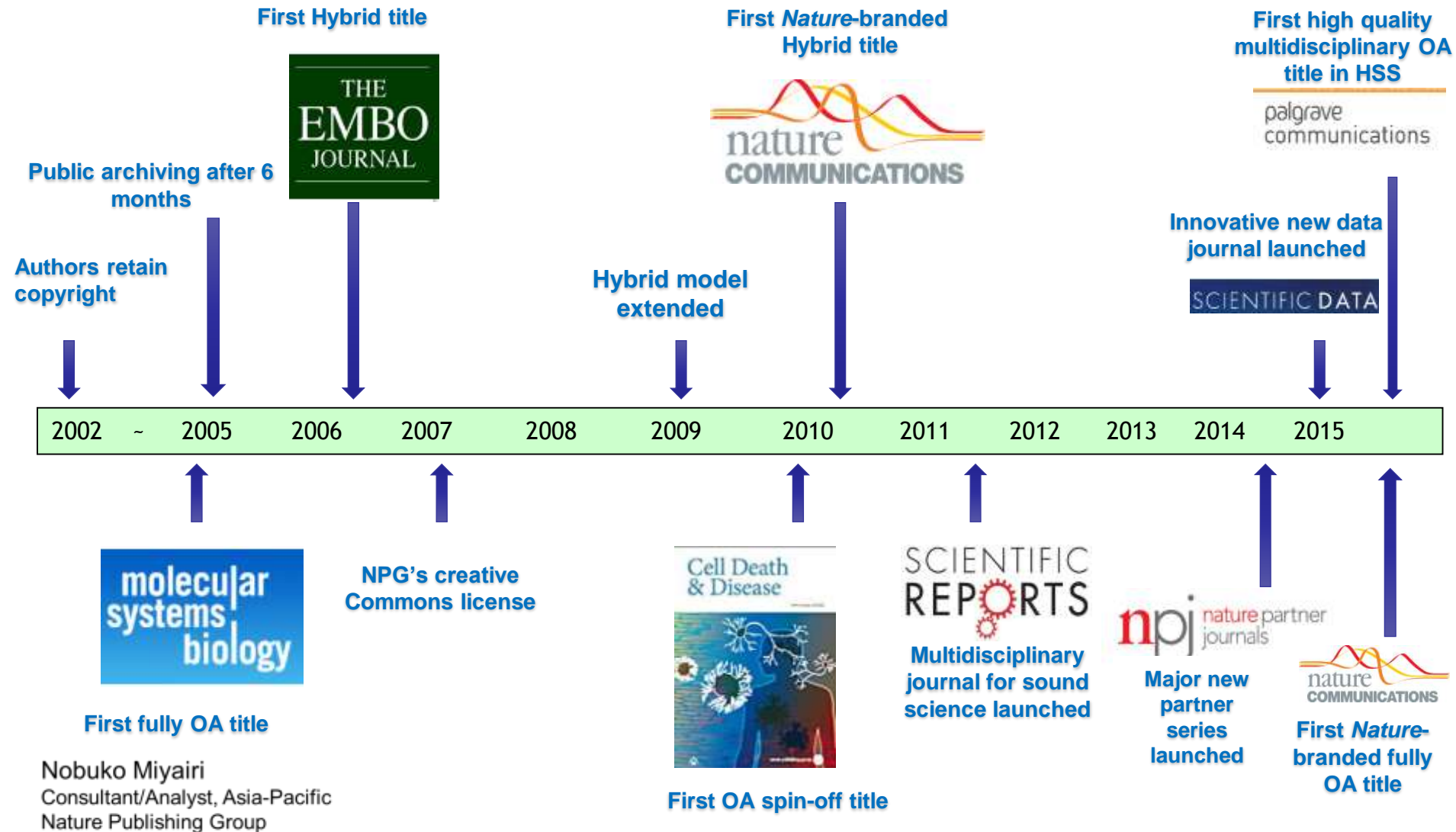
March 4, 2015

# Data journals



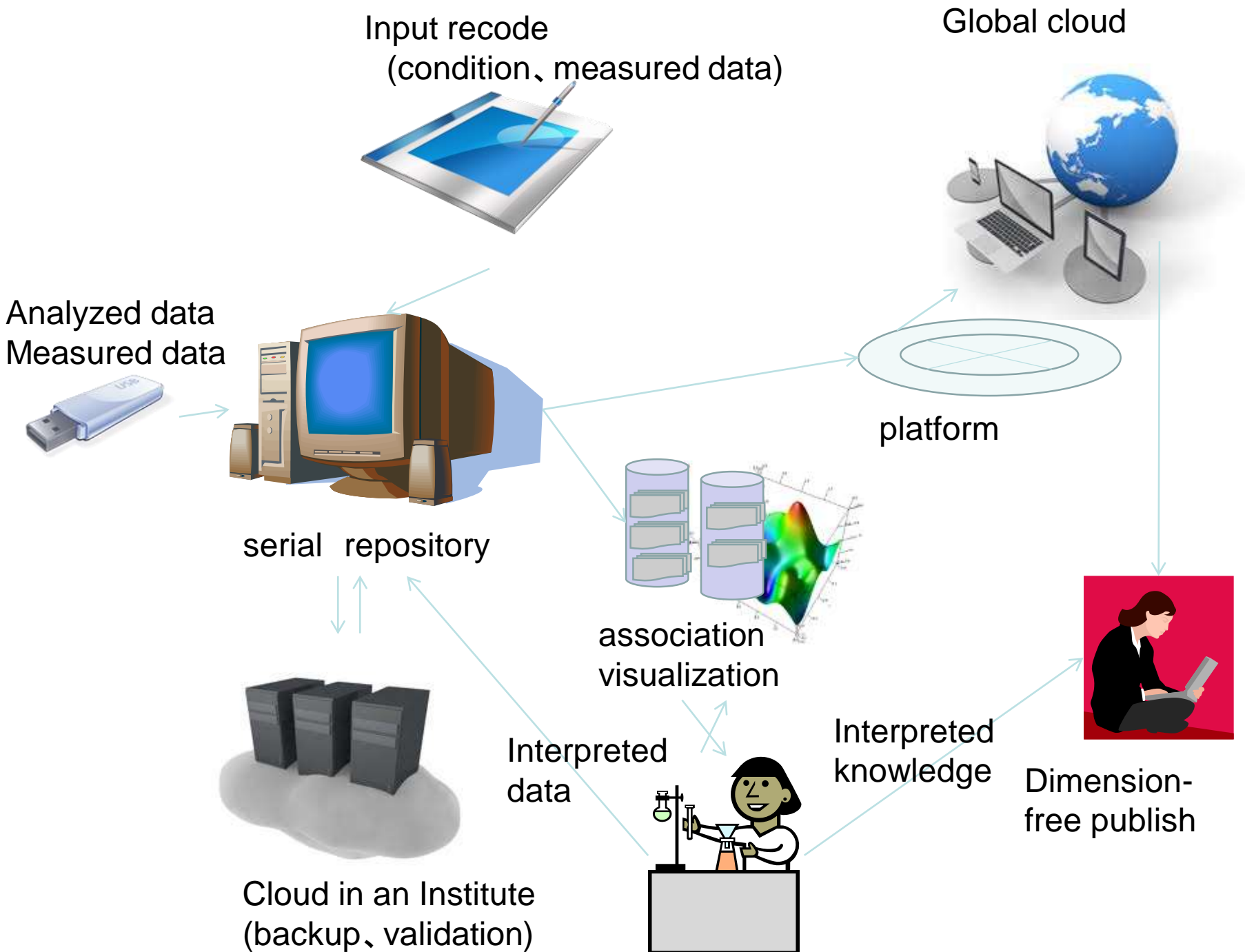


# Open Access (to research papers) at NPG

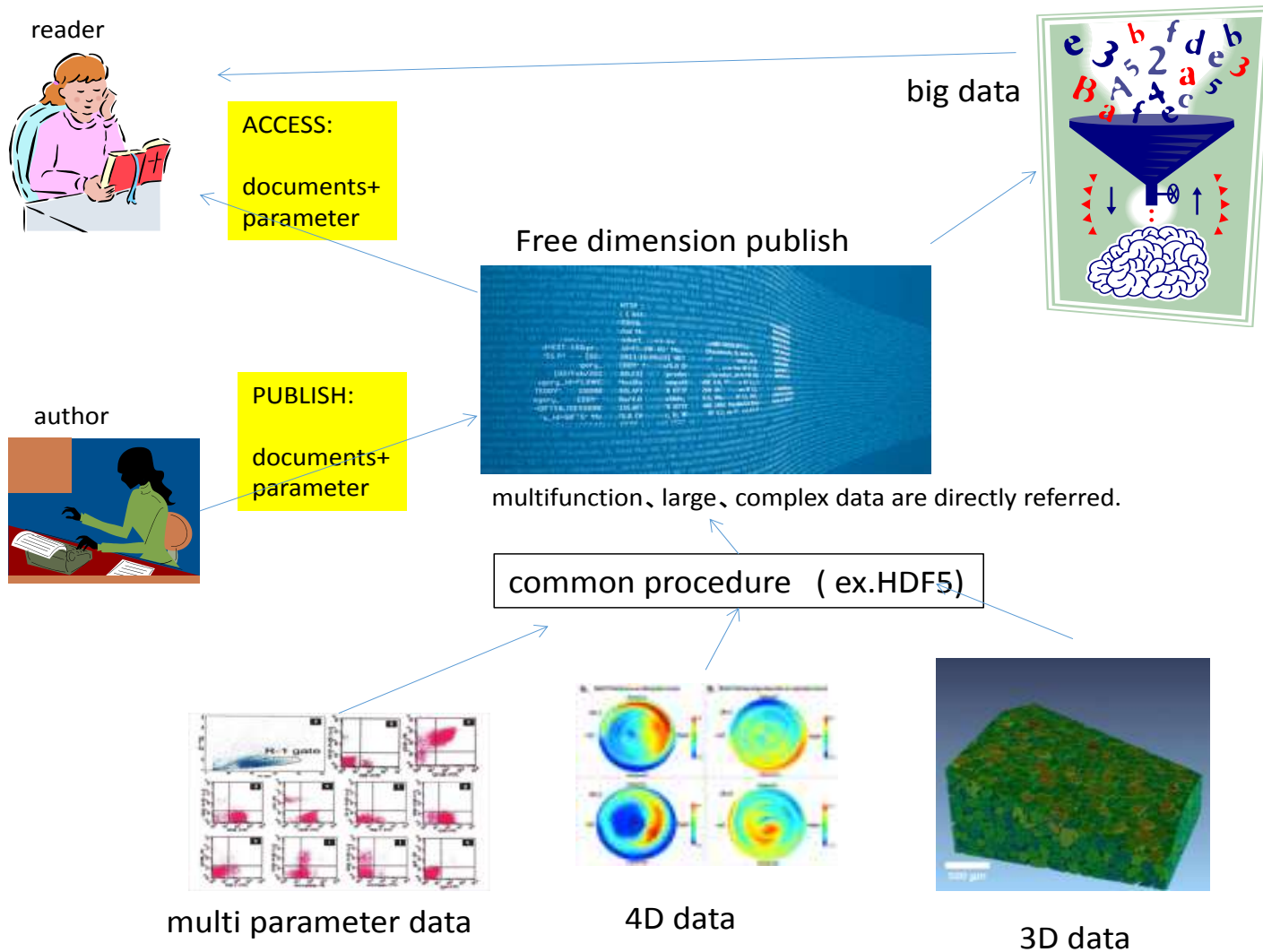


# Daily experimental note and institute cloud Only my proposal

- Every researcher takes note of experimental data.
- If we put them on data-space, it will make bigdata
- Software which helps easy data input is required.
- In an institute the data are stored in a cloud.
- It will be open after some period of time
  
- Data are not to be enclosed but its quality and the interpretation of author should be contended on open data.
- Reliability is not an attribute of datum, but interpretation.



# Material data should be shared beyond disciplines



# conclusion

- Material data in social space are optimistic
- Data in material space are pessimistic if architectures of database are discussed in a discipline.
- The effort to create bigdata is required.

Large Data sharing

Data Journal

Open data access

Daily experimental data note

Additive: Not only data but also knowledge should be distributed and accumulated.