DEVELOPING SIMULATION TOOLS FOR RESEARCH IN ALLOY DEFORMATION AND DEGRADATION

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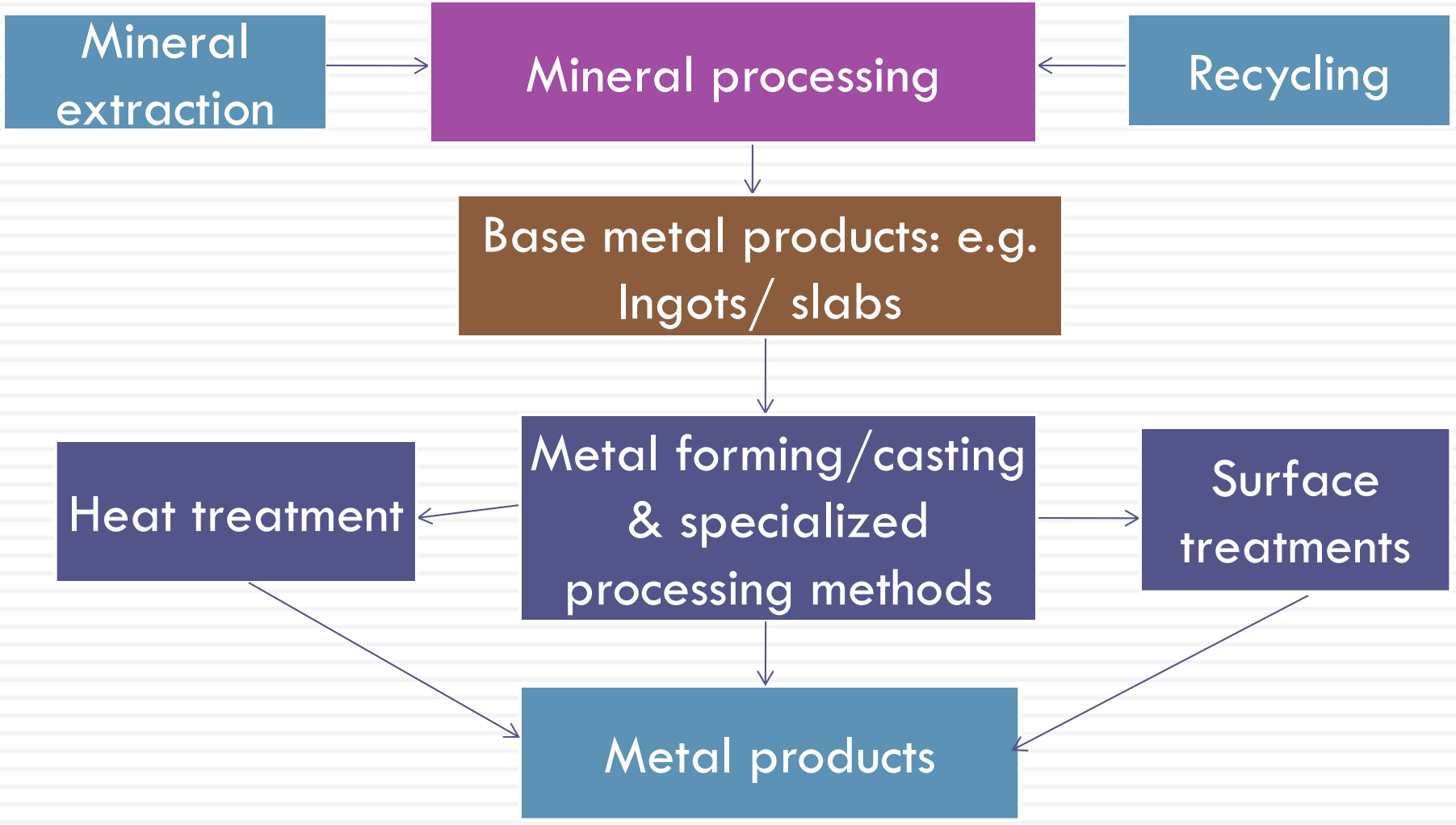
PROCESSING OF ALLOYS



PROCESSING AND APPLICATION NEEDS

A:

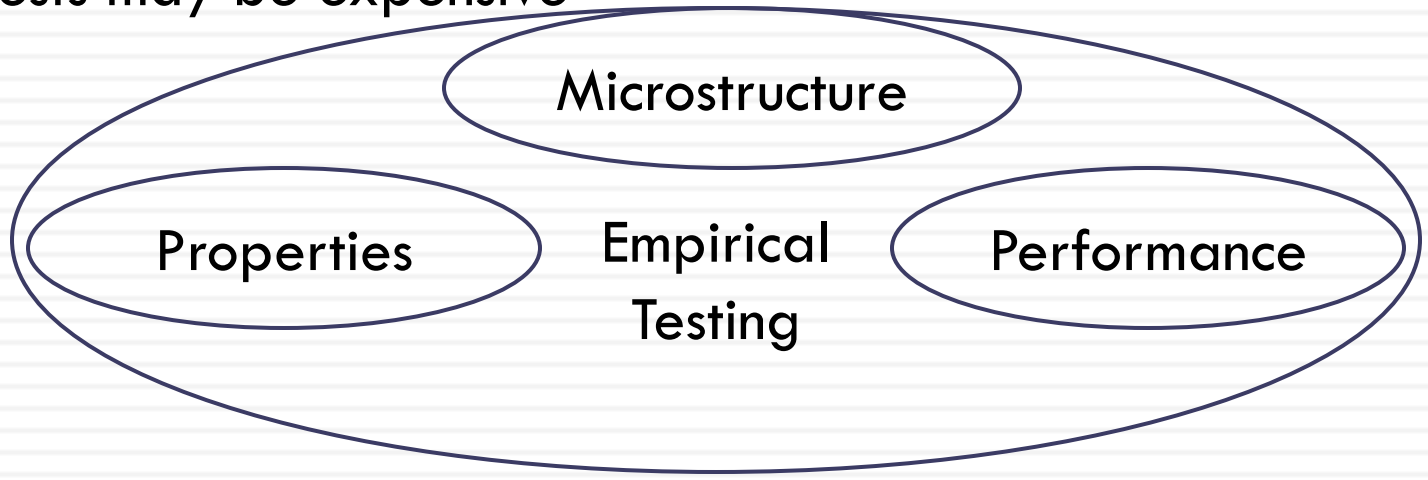
- Achievable melting points and lower energy consumption
- Controlled plastic flow during forming
- Techniques to enhance desired properties

B:

- Ability to forecast material properties – development and processing
- Ability to forecast component performance - application

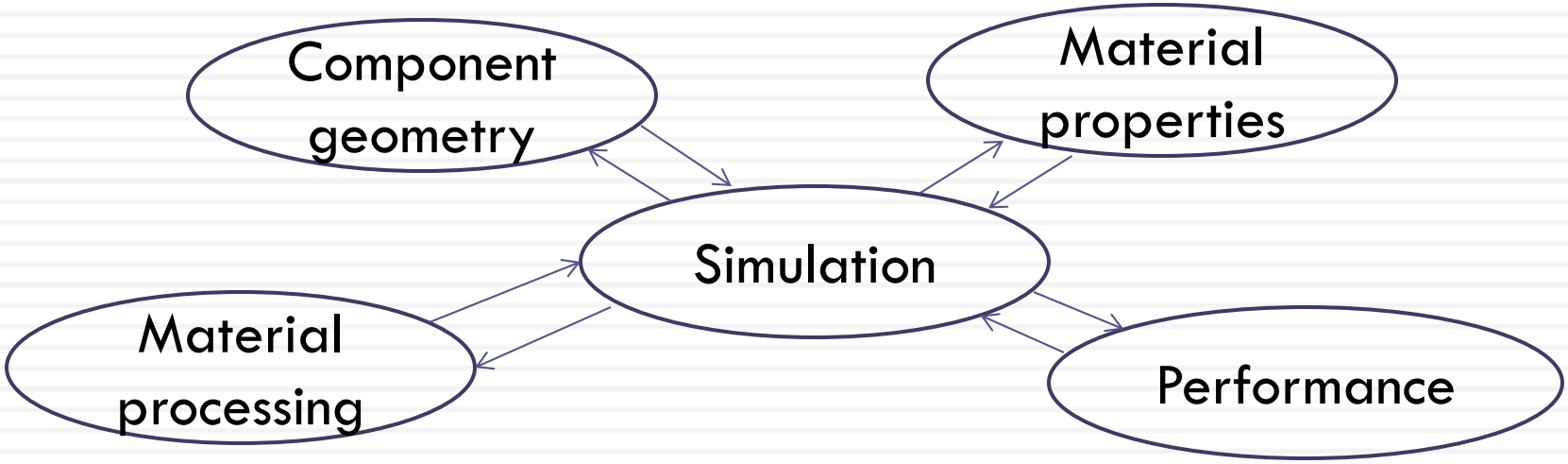
RATIONALE FOR ENGINEERING SIMMULATION - I

- Current approach: use empirical tests to generate data to enable one forecast behavior and performance;
  - Very effective
  - Requires specialized equipment – quite often high value
  - Tests may be expensive



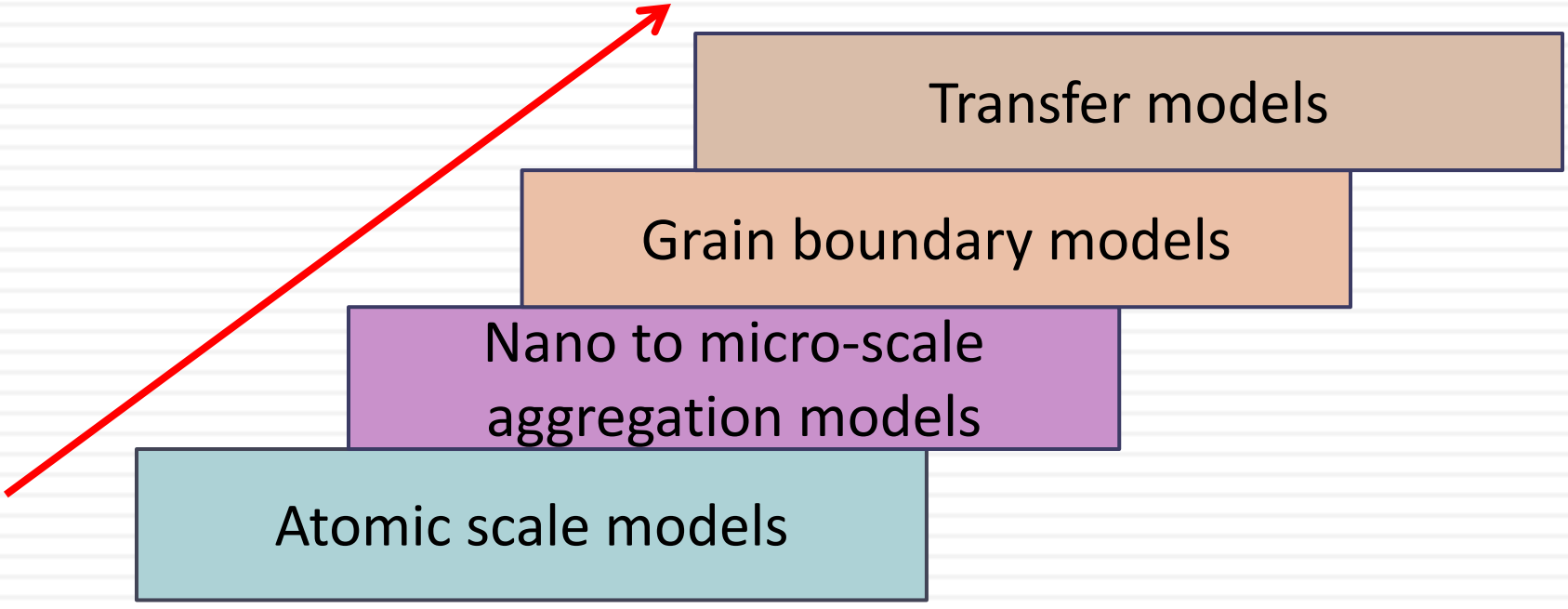
RATIONALE FOR ENGINEERING SIMMULATION - II

- New approach: use computers to simulate behavior;
  - Lower evaluation cost
  - A larger volume of data can be generated
  - Easily applied to the geometry of the part
  - Allows easy replacement of material



VALUE FOR MULTISCALE MATERIALS MODELING

- Eliminates the need to assume some underlying mechanism that drives the material's behavior



CHALLENGES TO SIMMULATION BASED RESEARCH

- Is limited to computational power and accuracy of scientific models used
- Requires development of simulation tools
- Needs validation using fundamental empirical data

CURRENT EFFORT

- Material is normally built by basic building blocks of differing sizes, shape, orientation and physical structure

- Need to establish mechanism for the interaction of building blocks – information required by the simulation tools

- Intervention – develop algorithms to manage the variation of the building blocks and the aggregation of their contribution.

OUR STRENGTHS

- Fundamentals and opportunities of multi-scale modeling using EAM are well understood
- Capacity to develop simulation code has been demonstrated
- 2 element BCC alloy - code developed. Can be enhanced to include:
  - More elements
  - FCC & HCP structures
- Capacity to develop models for simulation of material evolution has been demonstrated

OPPORTUNITIES

- Substantial foundational knowledge exists in micro/nano-scale materials evolution mechanisms
- Scalable architecture for a cluster HPC platform enables progressive investment
- Use collaboration to meet specialized validation efforts
- Pool of candidates for training in materials modeling

RESEARCH VISION

- Allow for variation in the alloy content
- Develop transferable models suitable for multi-element alloys
- Develop materials and engineering multi-scale simulation tools
- Apply simulation tools to study industry needs: e.g. roll forming, protection against corrosion, wear reduction, etc
- Develop a pool of competent computational materials scientists
- Develop computational materials modeling as a viable research technique for industrial development

CURRENT PROJECTS

- Simulation of Crack Propagation in a Pressure Vessels using the Energy J-Integral Method: J. K. Mutava, M.Sc. JKUAT
- Liner Wear Reduction in a Single Toggle Jaw crusher, G. Quartey, M.Sc. JKUAT
- Stress Analysis of Buried Oil Pipelines in Earthquake Prone Areas, L. Kikande, M.Sc. JKUAT

PROPOSED PROJECTS - I

- Corrosion modeling
  - Modeling of element contribution to corrosion resistance in nodular cast irons for the oil and gas industry valves and fittings
  - Modeling of corrosion mechanisms in sour gas oil pipelines
  - Modeling of corrosion mechanisms in construction steels for marine vessels
  - Modeling of corrosion mechanisms in rebar in water retention concrete structures
- Corrosion protection
  - Development of coatings for sour gas oil pipeline protection

PROPOSED PROJECTS - II

- DEM modeling of material flow & Wear modeling in the commutation processes, in selected mining equipment
- Variable roll forming
- Development of Ab-initio capacity

GROUP PHILOSOPHY