Lecture 6
Thermodynamics

PURDUE UNIVERSITY | Mechanical Engineering

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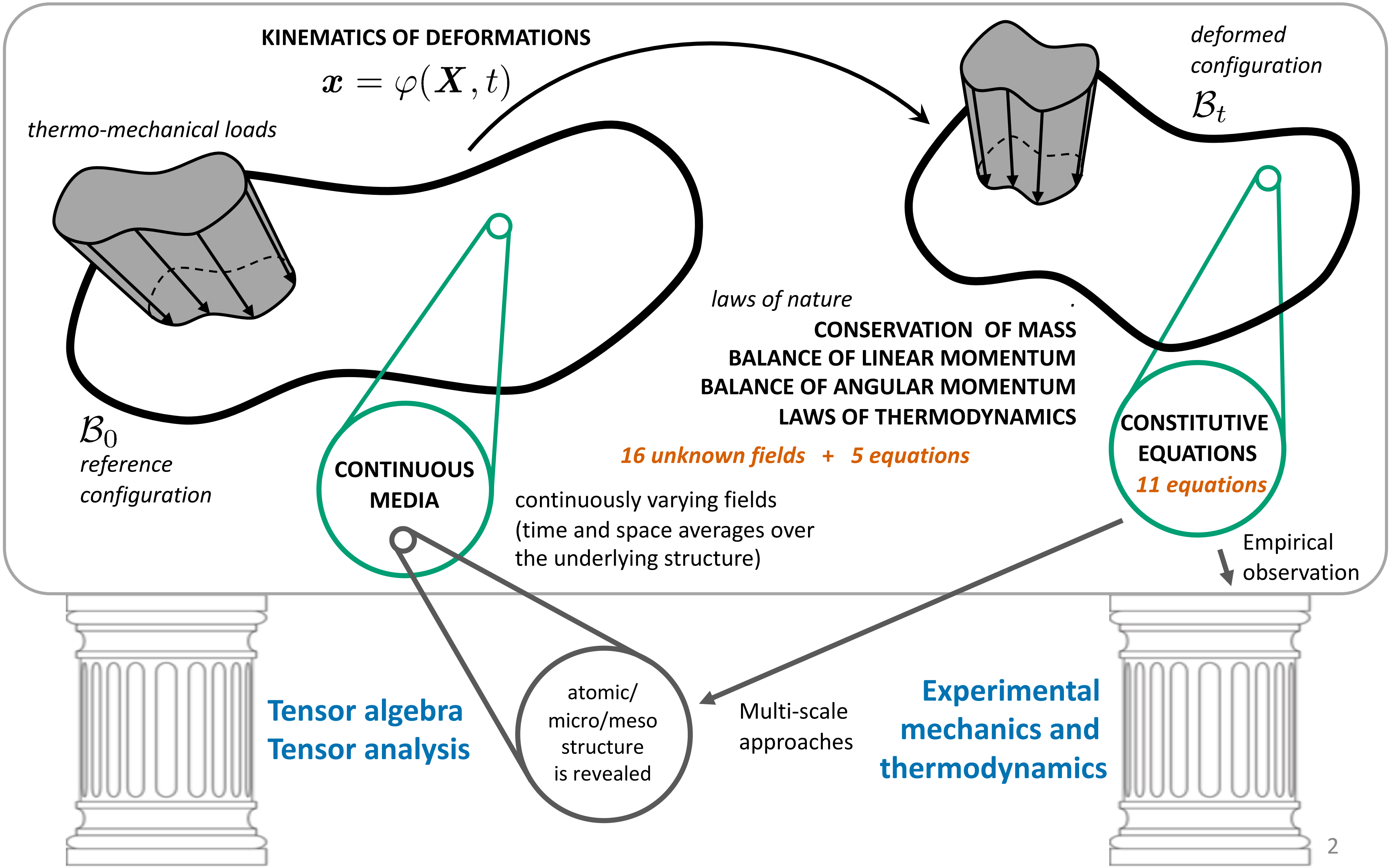
Lecture 6 – Thermodynamics



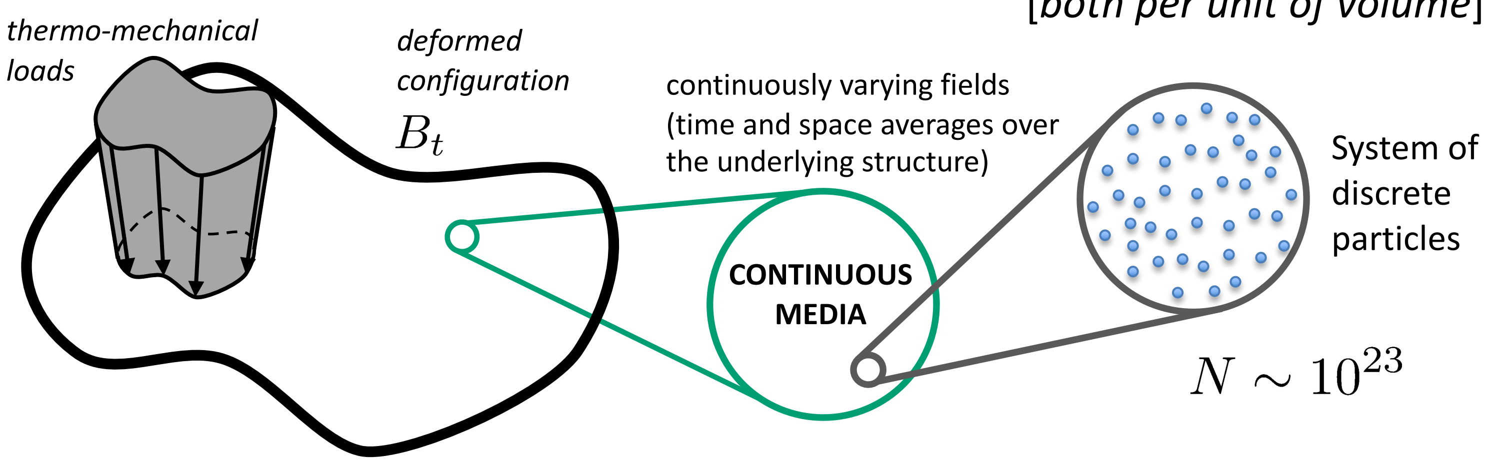
Thermodynamics

Macroscopic observable quantities

- Microscopic kinematics are described by a 6*N*-dimensional vector space (phase space) with all particle positions and momenta

$$\boldsymbol{y} = \{\boldsymbol{r}^1, \ldots, \boldsymbol{r}^N, m^1\dot{\boldsymbol{r}}^1, \ldots, m^N\dot{\boldsymbol{r}}^N\}$$

- Macroscopic kinematic quantities (e.g., total volume)
- Macroscopic non-kinematic quantities (e.g., total number of particles, total mass)
- Macroscopic fields (e.g., density, Lagrangian strain tensor) [*both per unit of volume*]



Thermodynamics

Thermodynamic equilibrium

After an external perturbation (of finite duration in time), all systems tend to evolve to a quiescent and spatially homogeneous (at the macroscopic length scale) terminal state where the system's macroscopic observables have constant limiting values.

State variables

Macroscopic observables that are well defined and single-valued when the system is at state of thermodynamic equilibrium.

Example: the thermodynamic equilibrium of a gas is characterized by the number of particles, the volume, the pressure and the temperature (i.e., 4 state variables).

Some state variables are kinematic state variables (such as volume and, for solids, strain). A change in a kinematic state variable results in a *thermodynamic tension*.

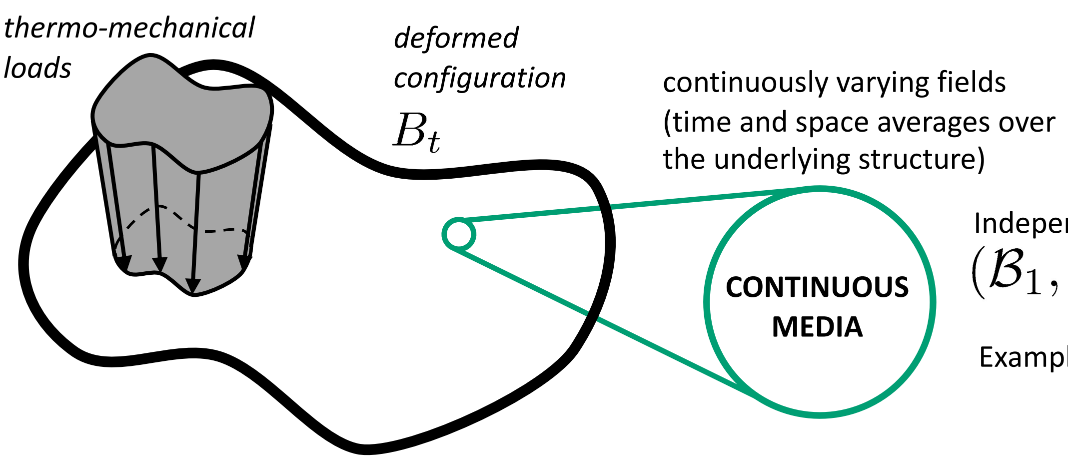
Thermodynamics

Laws of thermodynamics

- Zeroth law of thermodynamics $T \geq 0$ (…concept of absolute temperature)

- First law of thermodynamics $\mathcal{U}$ (…statement of conservation of energy)
  (…it leads to the idea of internal energy)

- Second law of thermodynamics (…directionality of thermodynamic processes)
  for an isolated system $\Delta\mathcal{S} \geq 0$ (…it leads of the idea of entropy)



Independent state variables
$(\mathcal{B}_1, \ldots, \mathcal{B}_{n^{\Gamma}+2})$

Example: $\boldsymbol{\Gamma} \cup (\mathcal{U}, \mathcal{S})$

Thermodynamics

(back to …) State variables

Any system in thermodynamic equilibrium is fully characterized by $n^{\boldsymbol{\Gamma}}+2$ independent state variables, where $n^{\boldsymbol{\Gamma}}$ is the number of independent kinematic state variables $\boldsymbol{\Gamma}=(\Gamma_1,\ldots,\Gamma_{n^{\boldsymbol{\Gamma}}})$ that characterize the system.

$$\boldsymbol{\mathcal{B}}=(\mathcal{B}_1,\ldots,\mathcal{B}_{n^{\boldsymbol{\Gamma}}+2},\ldots)$$

All state variables

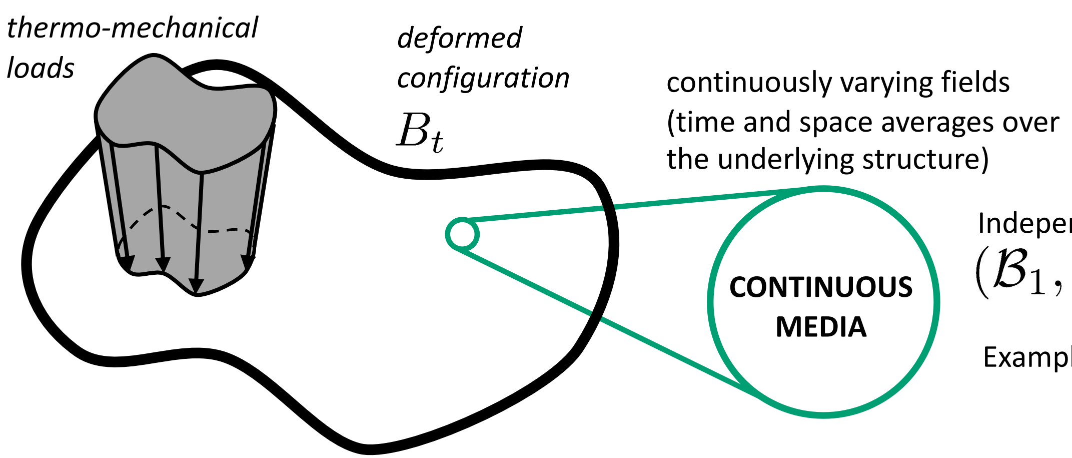
$$\mathcal{B}_{n^{\Gamma}+2+j}=f_j\left(\mathcal{U},\mathcal{S},\Gamma_1,\ldots,\Gamma_{n^{\Gamma}}\right)\qquad j=1,2,\ldots$$

Equations of state

Gas:

Solid:

DIY



Independent state variables

$$(\mathcal{B}_1,\ldots,\mathcal{B}_{n^{\boldsymbol{\Gamma}}+2})$$

Example: $\boldsymbol{\Gamma}\cup(\mathcal{U},\mathcal{S})$

Thermodynamics

Continuum thermodynamics

- Postulate of local thermodynamic equilibrium

  The local and instantaneous relations between thermodynamic quantities in a system out of equilibrium are the same as for a uniform system in equilibrium.

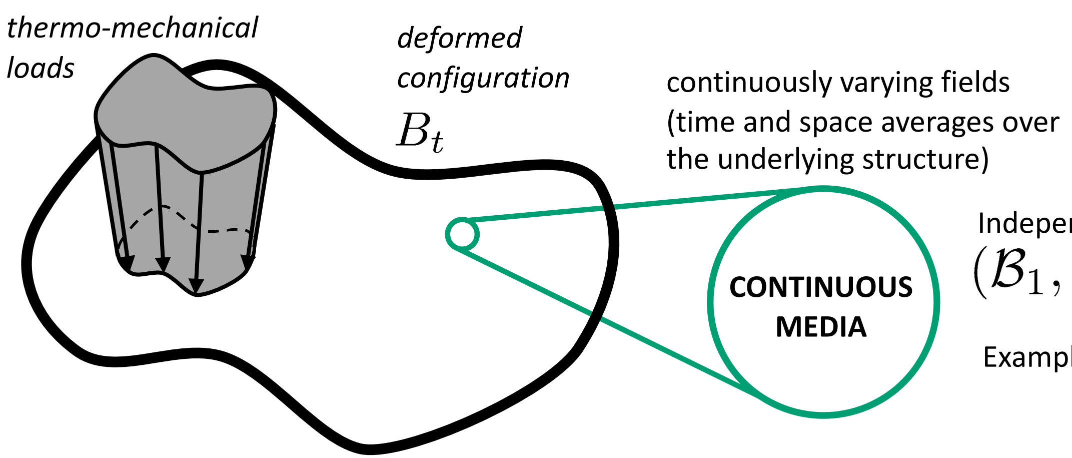
$$T \equiv T(\boldsymbol{x}, t)$$

$$p \equiv p(\boldsymbol{x}, t)$$

$$\rho \equiv \rho(\boldsymbol{x}, t)$$

$$u \equiv u(\boldsymbol{x}, t)$$ specific internal energy (internal energy per unit mass)

$$s \equiv s(\boldsymbol{x}, t)$$ specific entropy (entropy per unit mass)



Independent state variables

$$(\mathcal{B}_1, \ldots, \mathcal{B}_{n^{\Gamma}+2}) \equiv \boldsymbol{\mathcal{B}}(\boldsymbol{x}, t)$$

Example: $\boldsymbol{\Gamma} \cup (\mathcal{U}, \mathcal{S})$

Thermodynamics

Continuum thermodynamics

- First law of thermodynamics

$$\rho\dot{u} = \sigma_{ij}d_{ij} + \rho r - q_{i,i} \iff$$

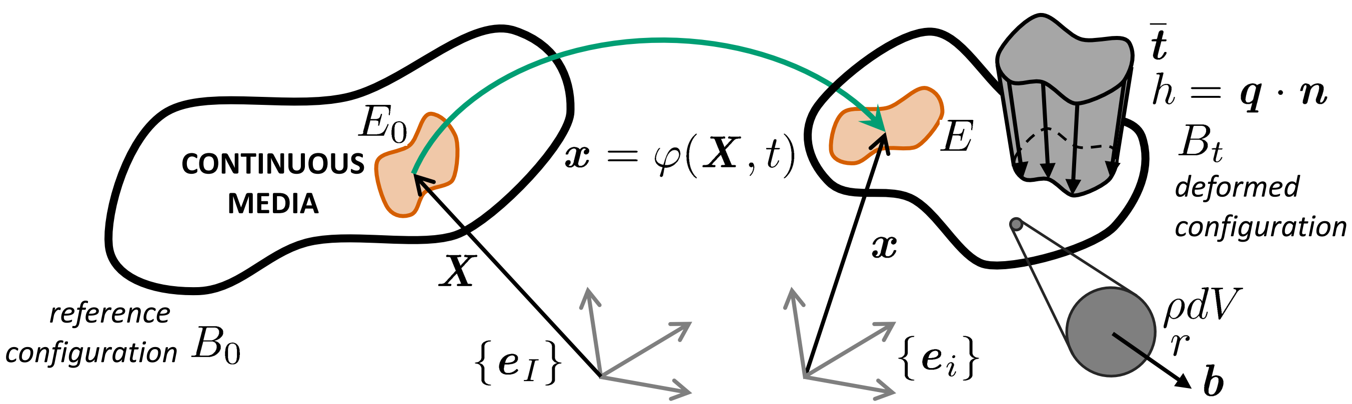
$$\rho\dot{u} = \boldsymbol{\sigma} : \boldsymbol{d} + \rho r - \mathrm{div}\boldsymbol{q} \qquad \forall \boldsymbol{x} \in B_t$$

spatial form of the conservation of energy

- Second law of thermodynamics

$$\dot{s} \geq \dot{s}^{\mathrm{ext}} = \frac{r}{T} - \frac{1}{\rho}\mathrm{div}\frac{\boldsymbol{q}}{T} \qquad \forall \boldsymbol{x} \in B_t$$

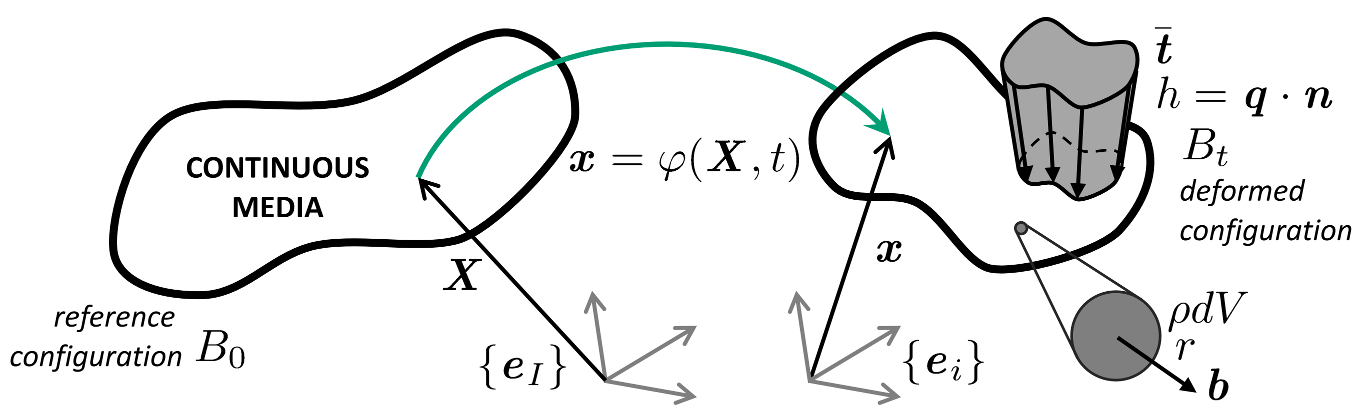
Clausius-Duhem inequality



Continuum mechanics – Laws of nature

Summary

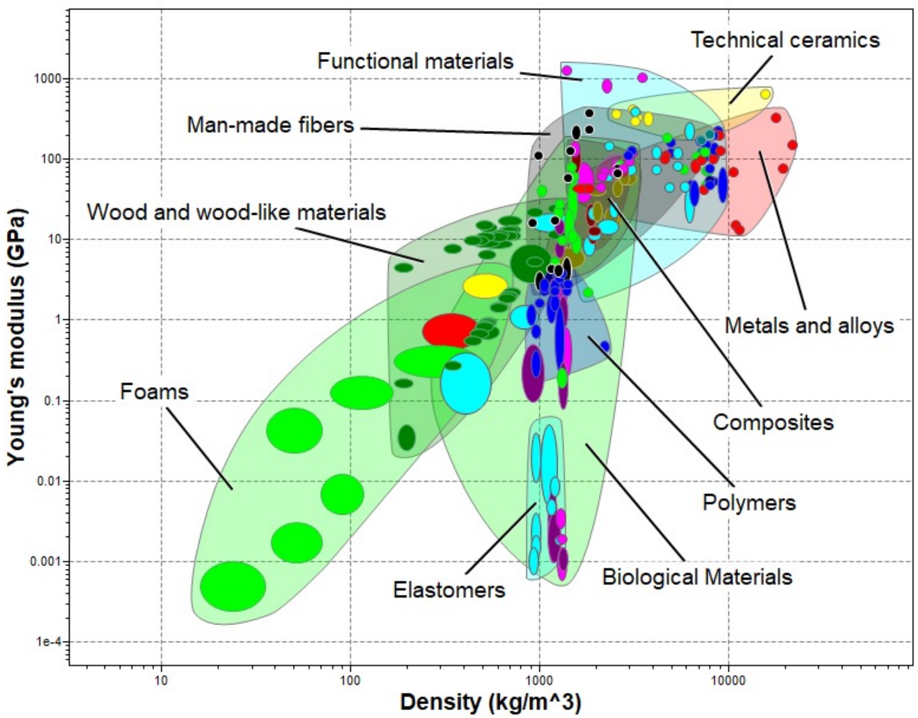
$J\rho = \rho_0$	$\forall \boldsymbol{X} \in B_0$	**conservation of mass**	(1 equation)
$\mathrm{div}\boldsymbol{\sigma} + \rho\boldsymbol{b} = \rho\boldsymbol{a}$	$\forall \boldsymbol{x} \in B$	**balance of linear momentum**	(3 equations)
$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$	$\forall \boldsymbol{x} \in B$	**balance of angular momentum**	(constraint)
$\rho\dot{u} = \boldsymbol{\sigma} : \boldsymbol{d} + \rho r - \mathrm{div}\boldsymbol{q}$	$\forall \boldsymbol{x} \in B$	**conservation of energy**	(1 equation)
$\dot{s} \geq \frac{r}{T} - \frac{1}{\rho}\mathrm{div}\frac{\boldsymbol{q}}{T}$	$\forall \boldsymbol{x} \in B$	**Clausius-Duhem inequality**	(constraint)
		$\rho,\ \boldsymbol{x},\ \boldsymbol{\sigma},\ \boldsymbol{q},\ u,\ s,\ T$	(16 unknowns)

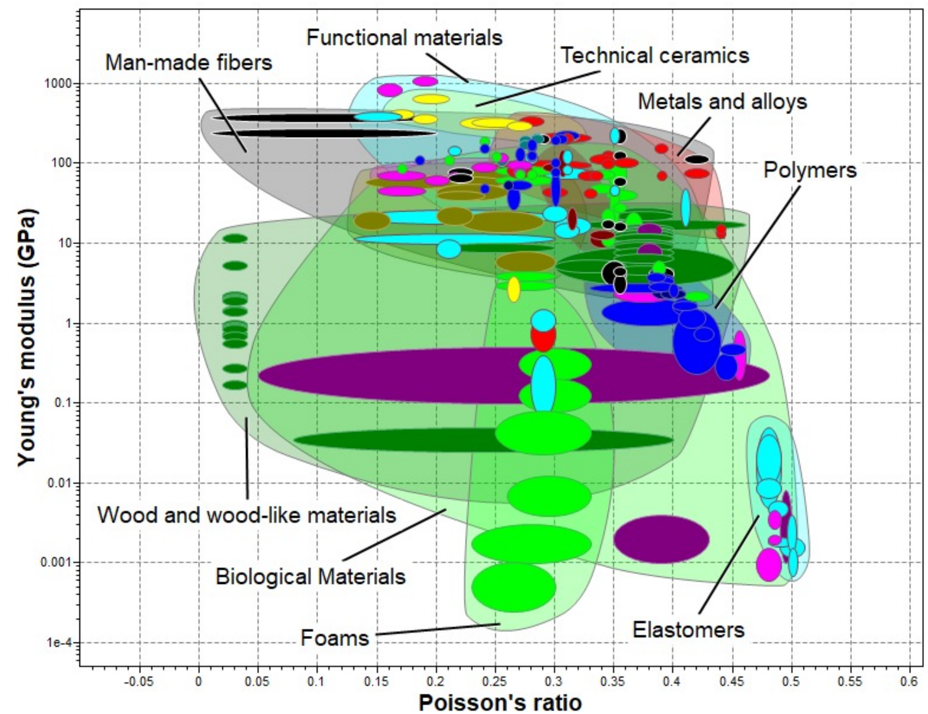


ME 597 – Solid Mechanics II (Ashby plots)

Young's modulus – Poisson's ratio – Density

- Flexible materials are typically light, and stiff materials are typically heavy.
- Polymers and elastomer are almost incompressible solids.
- Stiff lightweight materials are hard to find.

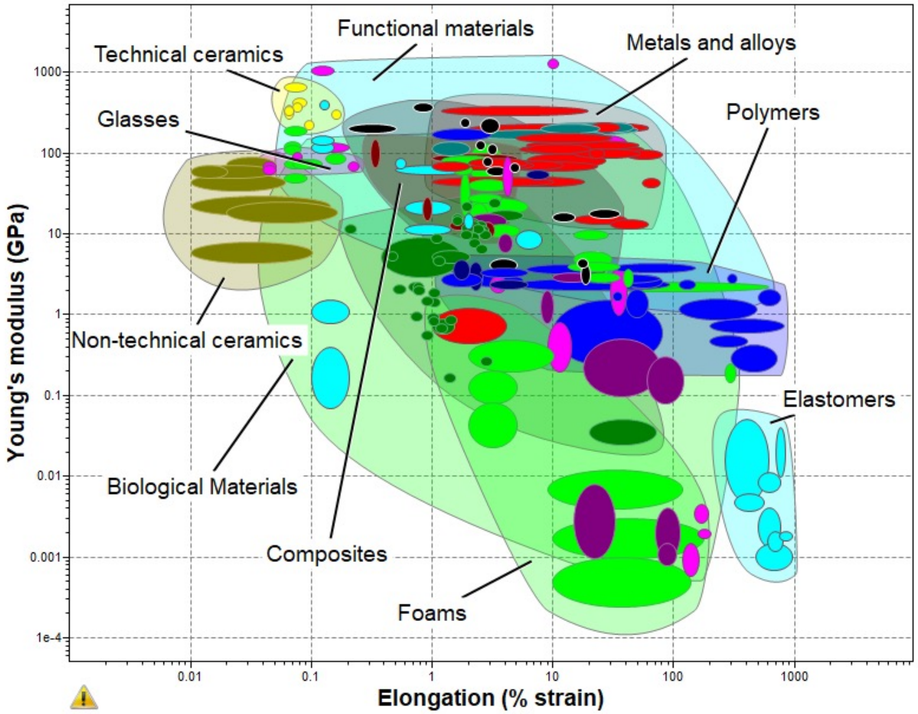


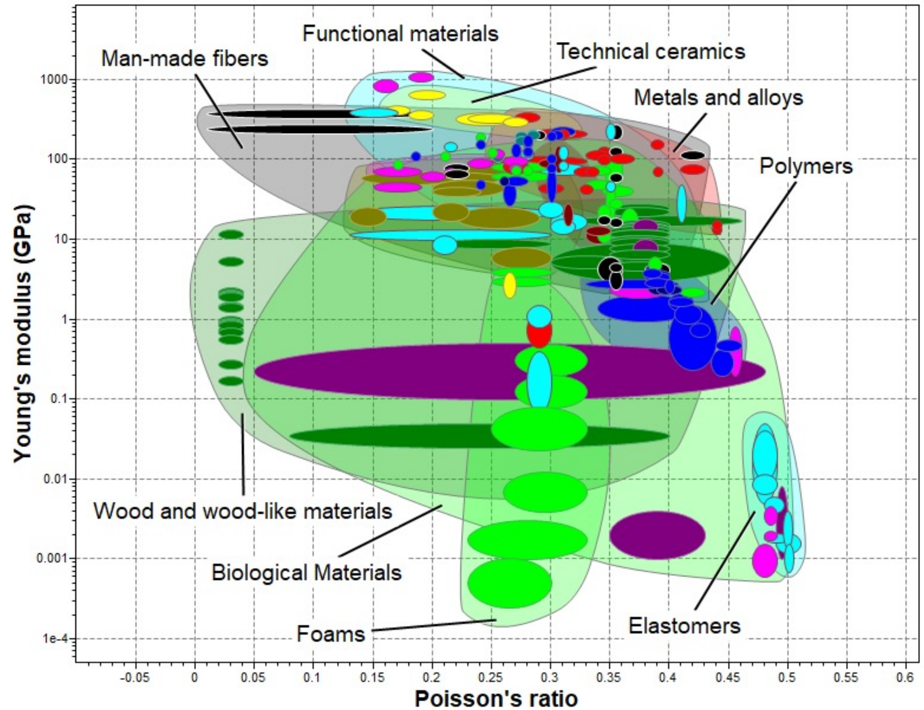


ME 597 – Solid Mechanics II (Ashby plots)

Young's modulus – Poisson's ratio – Elongation at failure

- Elastomers are polymers with viscoelasticity.
- Polymers and elastomers can exhibit elongations over 200%!
- Polymers and elastomer are almost incompressible solids.

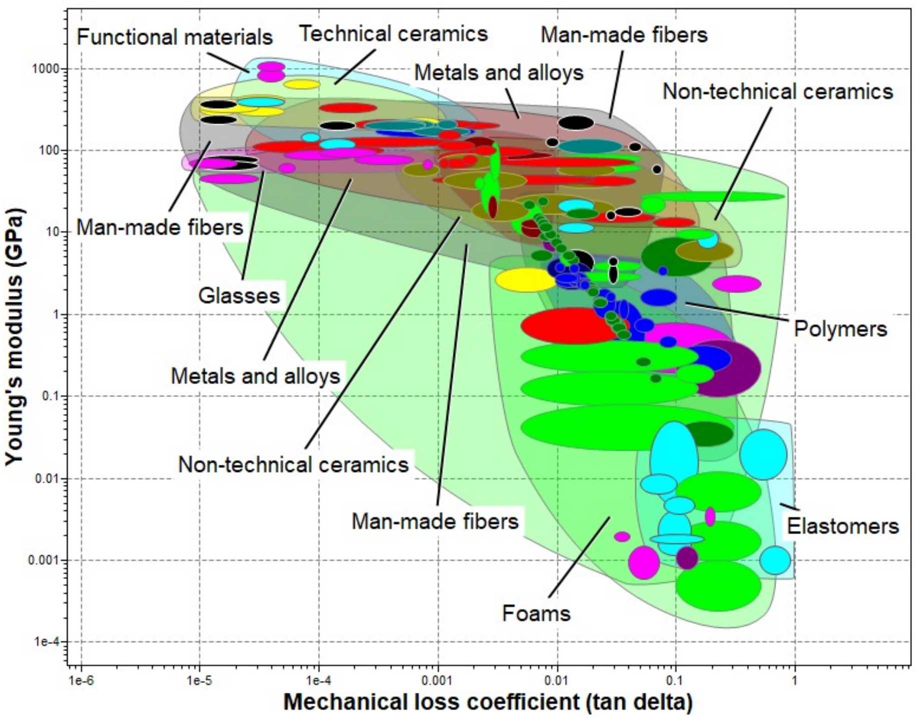


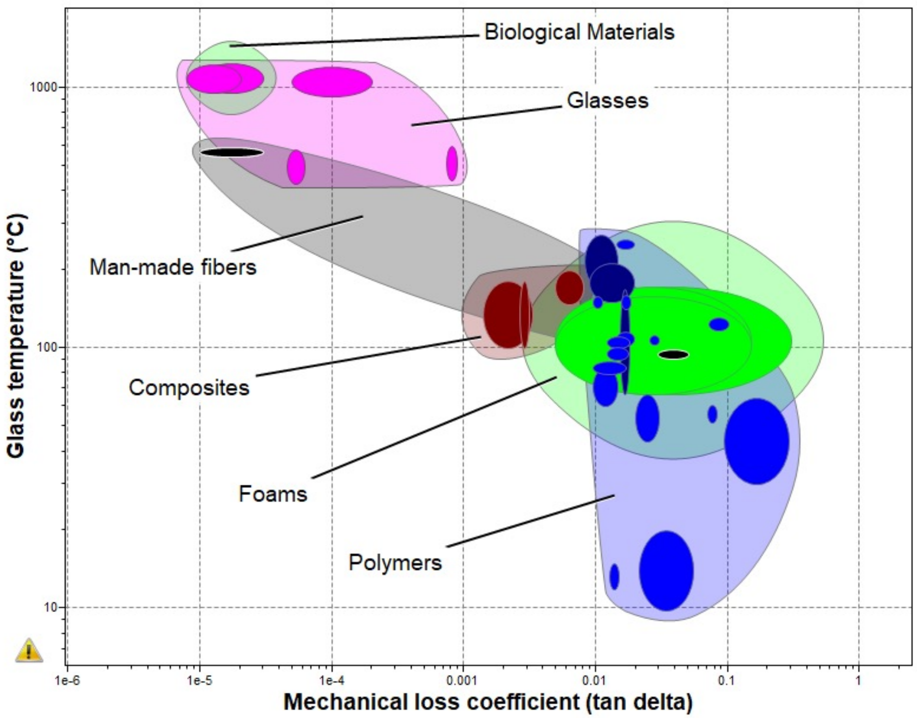


ME 597 – Solid Mechanics II (Ashby plots)

Young's modulus – Mechanical loss – Glass temperature

- Reversible transition from hard/brittle 'glassy' state into viscous state.
- Materials with good damping behavior (i.e., high vibrational energy dissipation) are typical soft and have low glass-transition temperatures.

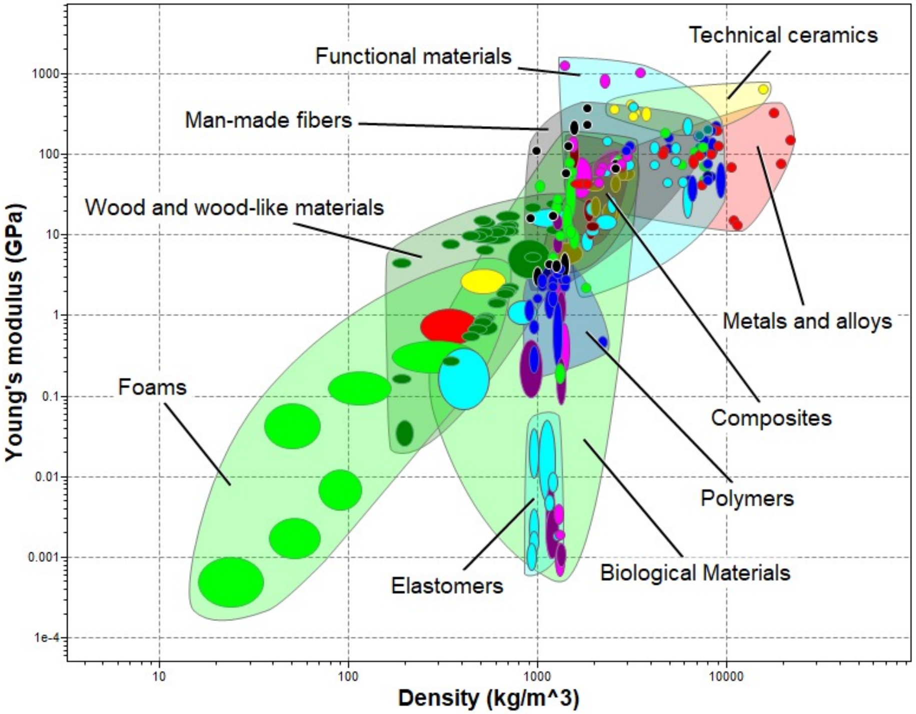


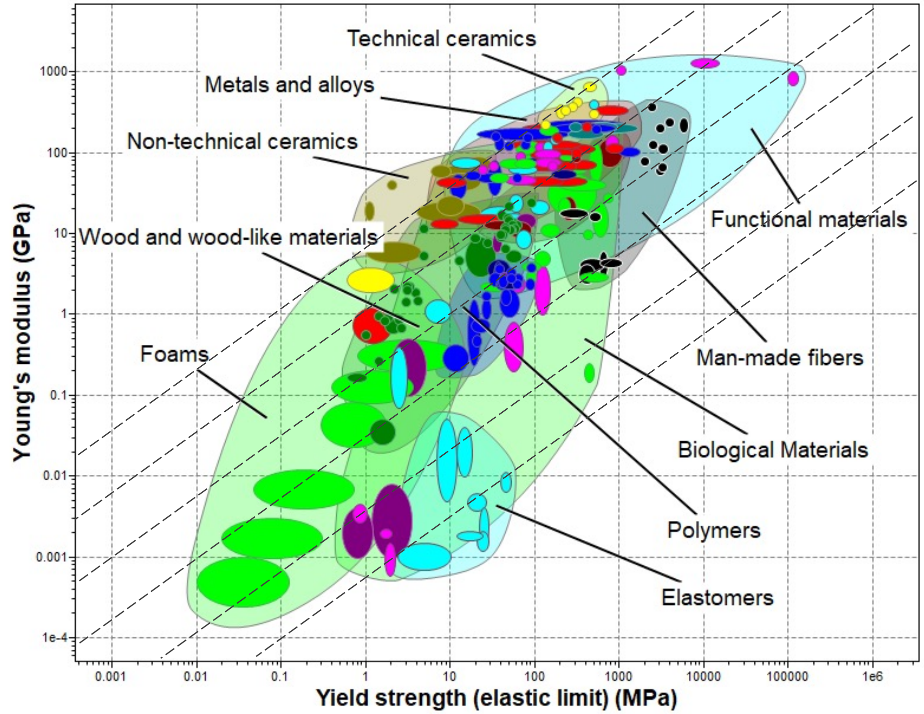


ME 597 – Solid Mechanics II (Ashby plots)

Young's modulus – Yield stress– Density

- Irreversible transition from elastic to plastic behavior.
- Contours of constant yield strain are a family of parallel lines on the Young's modulus vs. yield strength plot.





Any questions?