Multiscale Materials Modeling

Lecture 04

Capabilities of Continuum Modeling

Fundamentals of Sustainable Technology

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Capabilities of Continuum Modeling

I. What is Continuum Modeling?
II. Applications
    II.A. Continuum Mechanics
    II.B. Classical Electrodynamics
III. Numerical Techniques
    III.A. Finite Difference Methods
    III.B. Finite Element Methods
IV. Examples
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What is continuum modeling?

Continuum modeling is a term used to describe models of materials in which the discrete nature of matter and energy are not accounted for.

Frequently continuum modeling is considered “macroscopic” modeling, because in large systems one may be concerned about the distribution of kilograms of material rather than molecules of material.

Typically, the equations which describe the evolution of the mass, momentum and energy distributions are partial differential equations with their origin in classical physics.

Continuum modeling

<table>
<tr><td rowspan="4">Continuum mechanics
The study of the physics of continuous materials</td><td rowspan="2">Solid mechanics
The study of the physics of continuous materials with a defined rest shape.</td><td colspan="2">Elasticity
Describes materials that return to their rest shape after an applied stress.</td></tr>
<tr><td>Plasticity
Describes materials that permanently deform after a sufficient applied stress.</td><td rowspan="2">Rheology
The study of materials with both solid and fluid characteristics.</td></tr>
<tr><td rowspan="2">Fluid mechanics
The study of the physics of continuous materials which take the shape of their container.</td><td>Non-Newtonian fluids</td></tr>
<tr><td colspan="2">Newtonian fluids</td></tr>
</table>

http://en.wikipedia.org/wiki/Continuum_mechanics

We will present the governing equations for fluid mechanics first, then for solid mechanics.

They are identical in origin because they stem from conservation of mass, momentum and energy but they have different familiar forms due to different conventions and assumptions adopted for solid and fluid mechanics.

Continuum equations: mass balances

The continuity equation

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \left(\rho \mathbf{v}\right)$$

where ρ is the mass density, **v** is the center-of-mass velocity, and *t* is time. We understand very clearly that the LHS is an accumulation term and the right hand side is a convection term. The only assumption in equation (1) is that mass is not created or destroyed in the system, meaning that there are no nuclear reactions in our system. In Bird, Stewart and Lightfoot Second Edition (BSL2), this is equation (3.1-4) on page 77.

This equation expresses the physical law of conservation of mass.

Continuum equations: mass balances

Mass balance on a single component within a multicomponent system

$$\rho \frac{\partial w_A}{\partial t} = -\rho \mathbf{v} \cdot \nabla w_A - \nabla \cdot \mathbf{j}_A + \sum_{i=1}^{N_R} r_{i,A}$$

where w_A is the mass fraction of component A, $\mathbf{j}_A$ is the diffusive mass flux of component A relative to the center-of-mass velocity, N_R is the number of independent chemical reactions in the system, and $r_{i,A}$ is the rate of production of component A in reaction i, in units of mass/volume/time. The functional form of $\mathbf{j}_A$ depends on the choice of the form of the constitutive equation, i.e. Fick's law, that one chooses to employ. This diffusive flux can include the Soret effect, in which there is mass transfer due to a temperature gradient. We understand that the LHS is an accumulation term. The first term on the RHS is the convection term, the second term on the RHS is the diffusion term and the third term is the reaction term. Again, this equation neglects nuclear reaction. In BSL2, this is equation (19.1-14) on page 584.

This equation expresses the physical law of conservation of mass of a given species with the allowance that species can be generated and consumed via chemical reaction.

Continuum equations: momentum balances

The momentum balance typically has the form

$$\rho \frac{\partial \mathbf{v}}{\partial t} = -\rho \mathbf{v} \cdot \nabla(\mathbf{v}) - \nabla p - \nabla \cdot \boldsymbol{\tau} - \rho \nabla \hat{\Phi}$$

where p is the pressure, τ is the extra stress tensor, and $\hat{\Phi}$ is the specific external field imposed by, for example, gravity. If gravity is the source of the external field then we have $\mathbf{g} = -\nabla \hat{\Phi}$. Again, the functional form of the extra stress tensor must be determined by the choice of constitutive equation. One common constitutive equation is Newton's law of viscosity. We understand that the LHS is an accumulation term. The first term on the RHS is the convection term, the second term on the RHS represents the momentum transport due to molecular transport due to a gradient in the pressure, the third term is the momentum transport due to molecular transport due to viscous dissipation, and the fourth term is due to an external potential such as gravity. This equation is a the difference of equation (3.2-9) on page 80 of our textbook [1] and the continuity equation , equation(1). There are numerous assumptions in this equation. It assumes that there is no coupling of the momentum and reaction.

This equation expresses the physical law of conservation of momentum.

Continuum equations: energy balances

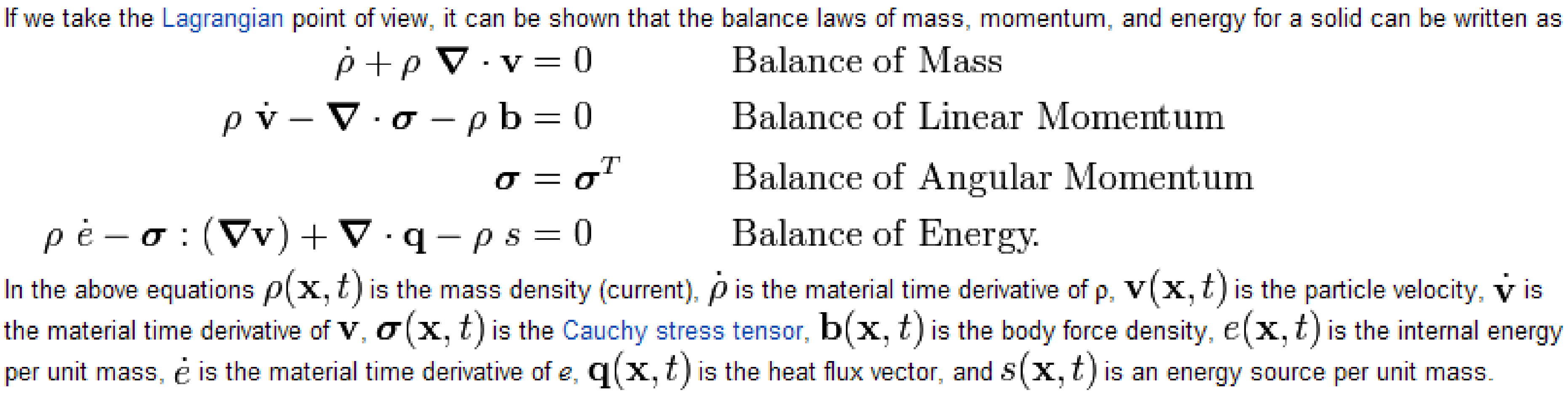
The total energy balance typically has the form

$$\frac{\partial \rho\left(\frac{1}{2}v^2 + \hat{U} + \hat{\Phi}\right)}{\partial t} = -\nabla \cdot \rho\left(\frac{1}{2}v^2\mathbf{v} + \hat{U}\mathbf{v} + \hat{\Phi}\mathbf{v}\right) - \nabla \cdot \mathbf{q} - \nabla \cdot p\mathbf{v} - \nabla \cdot \left(\boldsymbol{\tau} \cdot \mathbf{v}\right)$$

where $\hat{U}$ is the specific (per mass) internal energy, $\hat{\Phi}$ is the specific potential energy due to an external field, and **q** is the heat flux due to conduction. The term on the LHS is the accumulation term. The first term on the RHS is the convection term. The second term on the RHS is the conduction term. The third term on the RHS is the reversible rate of internal energy change per unit change in unit volume. Note that a compression will increase the internal energy. The last term on the RHS is the irreversible rate of internal energy increase per unit volume by viscous dissipation. This is equation (11.1-9) on page 336 in BSL2. We can add other terms to this energy balance to account for reactions and energy loss to the surroundings by other means.

This equation expresses the physical law of conservation of energy.

Solid mechanics



If we take the Lagrangian point of view, it can be shown that the balance laws of mass, momentum, and energy for a solid can be written as

$$\begin{aligned} \dot{\rho} + \rho\, \boldsymbol{\nabla} \cdot \mathbf{v} &= 0 && \text{Balance of Mass} \\ \rho\, \dot{\mathbf{v}} - \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} - \rho\, \mathbf{b} &= 0 && \text{Balance of Linear Momentum} \\ \boldsymbol{\sigma} &= \boldsymbol{\sigma}^T && \text{Balance of Angular Momentum} \\ \rho\, \dot{e} - \boldsymbol{\sigma} : (\boldsymbol{\nabla}\mathbf{v}) + \boldsymbol{\nabla} \cdot \mathbf{q} - \rho\, s &= 0 && \text{Balance of Energy.} \end{aligned}$$

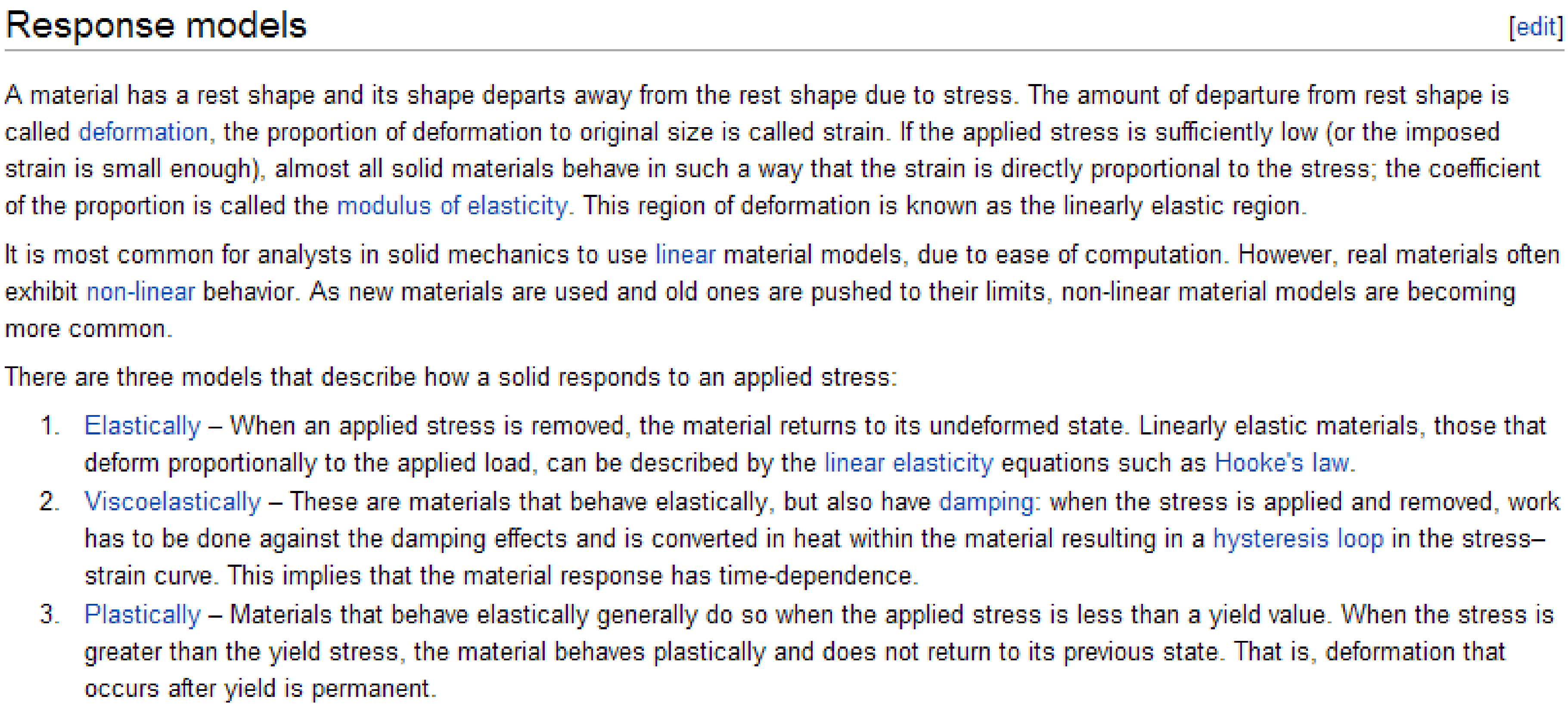
In the above equations $\rho(\mathbf{x},t)$ is the mass density (current), $\dot{\rho}$ is the material time derivative of ρ, $\mathbf{v}(\mathbf{x},t)$ is the particle velocity, $\dot{\mathbf{v}}$ is the material time derivative of $\mathbf{v}$, $\boldsymbol{\sigma}(\mathbf{x},t)$ is the Cauchy stress tensor, $\mathbf{b}(\mathbf{x},t)$ is the body force density, $e(\mathbf{x},t)$ is the internal energy per unit mass, $\dot{e}$ is the material time derivative of e, $\mathbf{q}(\mathbf{x},t)$ is the heat flux vector, and $s(\mathbf{x},t)$ is an energy source per unit mass.

http://en.wikipedia.org/wiki/Continuum_mechanics

These equations are of a form very similar to that shown for fluid mechanics. There are differences in convention however. For example, here the total stress tensor is used, rather than being divided into the pressure tensor and the extra stress tensor.

Continuum equations: solid mechanics

In solid mechanics the relationship between the applied stress and the resulting deformation (strain) is described by various response models that are inserted into the momentum and energy balances.



Response models

[edit]

A material has a rest shape and its shape departs away from the rest shape due to stress. The amount of departure from rest shape is called deformation, the proportion of deformation to original size is called strain. If the applied stress is sufficiently low (or the imposed strain is small enough), almost all solid materials behave in such a way that the strain is directly proportional to the stress; the coefficient of the proportion is called the modulus of elasticity. This region of deformation is known as the linearly elastic region.

It is most common for analysts in solid mechanics to use linear material models, due to ease of computation. However, real materials often exhibit non-linear behavior. As new materials are used and old ones are pushed to their limits, non-linear material models are becoming more common.

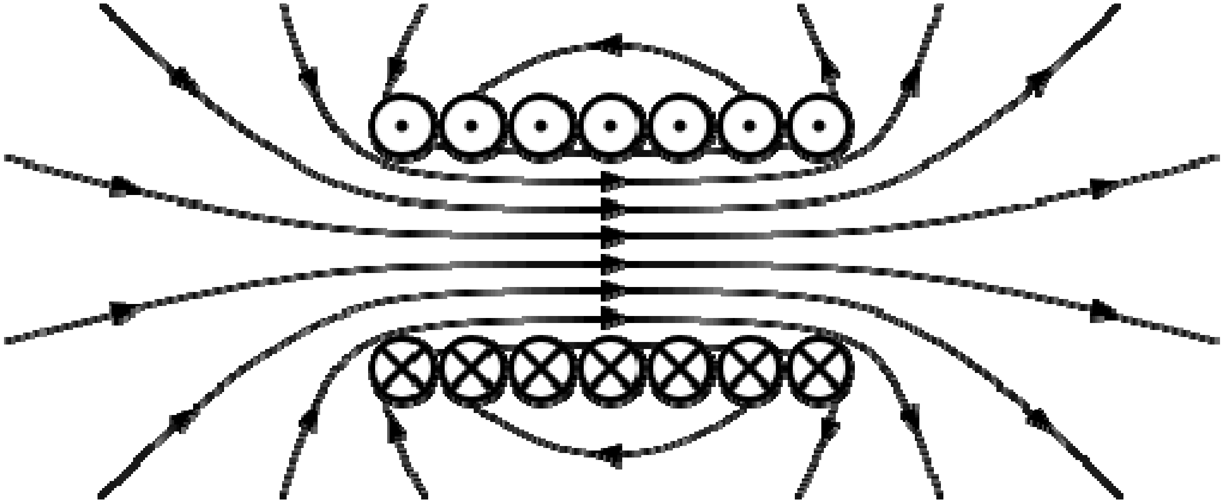
There are three models that describe how a solid responds to an applied stress:

1. Elastically – When an applied stress is removed, the material returns to its undeformed state. Linearly elastic materials, those that deform proportionally to the applied load, can be described by the linear elasticity equations such as Hooke's law.
2. Viscoelastically – These are materials that behave elastically, but also have damping: when the stress is applied and removed, work has to be done against the damping effects and is converted in heat within the material resulting in a hysteresis loop in the stress–strain curve. This implies that the material response has time-dependence.
3. Plastically – Materials that behave elastically generally do so when the applied stress is less than a yield value. When the stress is greater than the yield stress, the material behaves plastically and does not return to its previous state. That is, deformation that occurs after yield is permanent.

http://en.wikipedia.org/wiki/Solid_mechanics

Continuum equations: electromagnetism

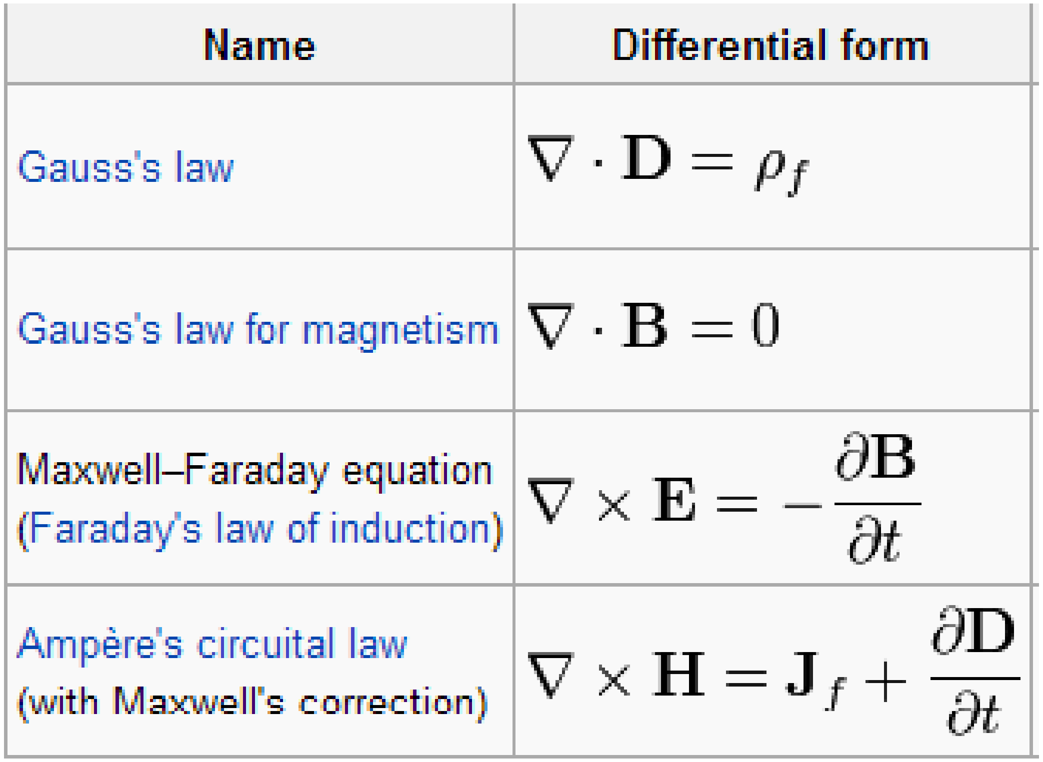
The theory of classical electromagnetism is also evaluated via continuum models.



http://en.wikipedia.org/wiki/Electrodynamics

Continuum equations: classical electrodynamics

Modeling classical electrodynamics requires Maxwell's Equations



Name	Differential form
Gauss's law	$\nabla \cdot \mathbf{D} = \rho_f$
Gauss's law for magnetism	$\nabla \cdot \mathbf{B} = 0$
Maxwell–Faraday equation (Faraday's law of induction)	$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$
Ampère's circuital law (with Maxwell's correction)	$\nabla \times \mathbf{H} = \mathbf{J}_f + \frac{\partial \mathbf{D}}{\partial t}$

http://en.wikipedia.org/wiki/Maxwell%27s_equations

E – electric field
B – magnetic field
D – electric displacement field
H – magnetizing field
ρ_f – free charge density
J_f – free current density
q – charge
v – velocity

and requires Lorentz's force law

$$\mathbf{F} = q[\mathbf{E} + (\mathbf{v} \times \mathbf{B})],$$

Constitutive Equations

Conservation laws describe laws of physics but do not instrinsically provide material properties. For fluid mechanics describing an N-component fluid in d-dimensional space, we have N + d + 1 equations. There are N mass balances, d momentum balances (one for each relevant component, x, y and z) and one energy balance. These equations yield the solutions to N + d + 1 variables: the density, the mass fraction of each species, the velocities and the temperature.

Any other variable in the equations must be input, including

- pressure
- diffusive flux (e.g. Fick's law)
- reaction rate laws
- extra stress tensor (e.g. Newton's law of viscosity)
- body forces
- internal energy
- heat conductive flux (e.g. Fourier's law)

All of these properties are either functions of the variables (density, composition, velocity, temperature) or constants. For example, pressure requires an equation of state providing the pressure in terms of the density, composition and temperature. The fluxes require diffusion coefficients, viscosities or thermal conductivities. These are inputs to continuum models and not outputs.

Outline

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Continuum Modeling: equations types

All of the governing equations in fluid and solid mechanics are partial differential equations because the unknown variables, density, velocity, temperature are functions of more than one variable: time (t) and space (x,y and z).

Moreover, these equations are parabolic partial differential equations because they are have first order derivatives in time and second order derivatives in space. In general a parabolic PDE has the form

$$\frac{\partial f(x,y,z,t)}{\partial t} = G\left[f(x,y,z,t), \nabla f(x,y,z,t), \nabla^2 f(x,y,z,t)\right]$$

where G is some operator (linear or nonlinear). Example:

$$\rho\frac{\partial w_A}{\partial t} = -\rho\mathbf{v}\cdot\nabla w_A - \nabla\cdot\mathbf{j}_A + \sum_{i=1}^{N_R} r_{i,A} \qquad \text{(mass balance on species A)}$$

$$\mathbf{j}_A = -\rho D\nabla w_A \qquad \text{(Fick's law for isothermal, binary system)}$$

$$\rho\frac{\partial w_A}{\partial t} = -\rho\mathbf{v}\cdot\nabla w_A + \nabla\rho D\cdot\nabla w_A + \rho D\nabla^2 w_A + \sum_{i=1}^{N_R} r_{i,A} \qquad \text{(parabolic PDE)}$$

Continuum Modeling: equations types

At steady state, the time derivatives may be considered zero and all of the material, momentum and energy balances become elliptic PDEs. In other words, none of the unknown variables are functions of time. In general a parabolic PDE has the form

$$0 = G\left[f(x,y,z,t), \nabla f(x,y,z,t), \nabla^2 f(x,y,z,t)\right]$$

where G is some operator (linear or nonlinear). Example:

transient mass balance on species A (parabolic PDE)

$$\rho \frac{\partial w_A}{\partial t} = -\rho \mathbf{v} \cdot \nabla w_A + \nabla \rho D \cdot \nabla w_A + \rho D \nabla^2 w_A + \sum_{i=1}^{N_R} r_{i,A}$$

steady state mass balance on species A (elliptic PDE)

$$0 = -\rho \mathbf{v} \cdot \nabla w_A + \nabla \rho D \cdot \nabla w_A + \rho D \nabla^2 w_A + \sum_{i=1}^{N_R} r_{i,A}$$

In the event that there was only one spatial dimension, the steady state equation becomes an ordinary differential equation.

$$0 = -\rho v \frac{dw_A}{dz} + \frac{d\rho D}{dz} \frac{dw_A}{dz} + \rho D \frac{d^2 w_A}{dz^2} + \sum_{i=1}^{N_R} r_{i,A}$$

Handling time evolution

In the numerical solution of differential equations, we discretize the function, meaning we approximate the continuous function by evaluating it at a set of discrete points. For an ordinary differential equation, in which the unknown is a function of only one independent variable, we have a problem statement with the equation and an initial condition.

$$\frac{df(t)}{dt} = g(f,t) \qquad f(t = t_o) = f_o$$

The simplest numerical solution is a first order approximation, Euler's method,

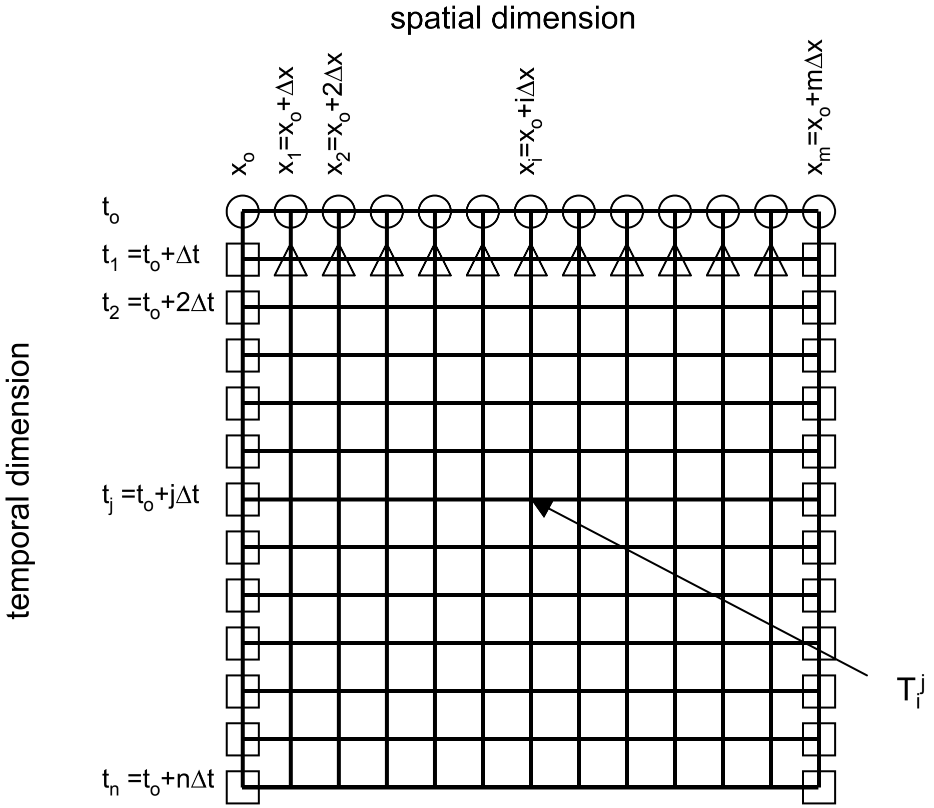
$$\frac{df(t)}{dt} \approx \frac{f(t_{i+1}) - f(t_i)}{t_{i+1} - t_i} = g\left(f(t_i), t_i\right)$$

Rearrangement yields

$$f(t_{i+1}) = f(t_i) + (t_{i+1} - t_i)\,g\left(f(t_i), t_i\right)$$

Thus one can start at the initial condition, evaluate *g* and step along in time for an arbitrary number of steps (typically until the system has reached a steady state). This is how time is handled. Although, higher order more accurate methods than the Euler method are usually employed. Spatial derivatives are handled a different way.

Finite Difference: space



legend

○ node where temperature is known due to initial condition

□ node where temperature is known due to boundary condition

△ node where temperature is unknown but will be solved for

For PDEs with spatial derivatives, we discretize the spatial dimensions and use finite difference formulas to eliminate all spatial derivatives.

First derivative

$$\left(\frac{\partial T}{\partial x}\right)_i^j \approx \frac{T_{i+1}^j - T_{i-1}^j}{x_{i+1} - x_{i-1}}$$

Second derivative

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_i^j \approx \frac{T_{i+1}^j - 2T_i^j + T_{i-1}^j}{\Delta x^2}$$

In this manner, a parabolic PDE is converted to a set of coupled ODEs (time derivatives only) and can be solved as shown on the previous slide.

Elliptic PDEs (steady state) are converted into a set of algebraic equations.

Finite Elements: space

In finite elements, for elliptic (steady state) PDEs

1. the PDEs are first analytically converted into integral equations.
2. a grid over the spatial domain is generated, perhaps nonuniform, if the solution is expected to contain steep slopes in some areas and gentle slopes in others.
3. The solution is formulated as a linear combination of simple (typically polynomial) functions (the basis set).
4. The unknowns are now simply the coefficients of the basis set at each point.
5. The discretized integrals are converted into a system of algebraic equations, which is solved using linear algebra.

Finite Elements: space

Problem statement as PDE.

$$u''(x) = f(x) \text{ in } (0,1),$$
$$u(0) = u(1) = 0,$$

Convert to integral form (weak form).

$$\int_0^1 f(x)v(x)\,dx = \int_0^1 u''(x)v(x)\,dx. = -\int_0^1 \underline{u'(x)v'(x)\,dx}$$

Define basis functions. (piecewise linear here)

$$v_k(x) = \begin{cases} \frac{x-x_{k-1}}{x_k - x_{k-1}} & \text{if } x \in [x_{k-1}, x_k], \\ \frac{x_{k+1} - x}{x_{k+1} - x_k} & \text{if } x \in [x_k, x_{k+1}], \\ 0 & \text{otherwise}, \end{cases}$$

Solution is linear combination of basis functions.
(Now the set of u_k are the unknowns.)

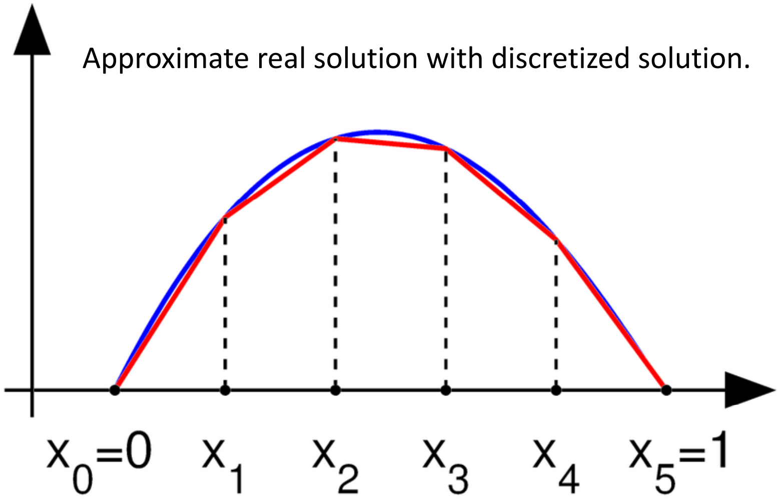
$$u(x) = \sum_{k=1}^{n} u_k v_k(x)$$

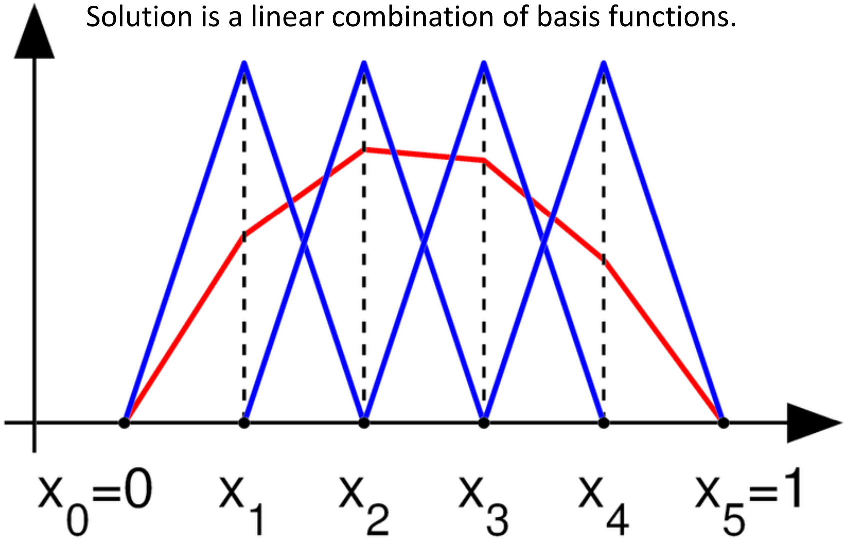
Integration of simple basis functions is easy.

$$\phi(v_j, v_k) = \int_0^1 v_j' v_k'\,dx$$

$$-\sum_{k=1}^{n} u_k \phi(v_k, v_j) = \sum_{k=1}^{n} f_k \int v_k v_j dx \text{ for } j = 1,\dots,n. \quad (4)$$

Use linear algebra to solve for u_k .


Approximate real solution with discretized solution.


Solution is a linear combination of basis functions.

http://en.wikipedia.org/wiki/Finite_element_method

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Strengths and Weaknesses

Advantages:
Coarse-grained models provide the opportunity to capture behavior on large length and time scales. By integrating coarse-grained models with more finely resolved models, one can develop high-fidelity models with atomic details applied to macroscopic time and length scales.

Disadvantages:

- Coarse-grained models gain an advantage by dropping some physics. If you remove important physics, your model will not give accurate results.
- Coarse-grained models require parameterization from more finely resolved models.