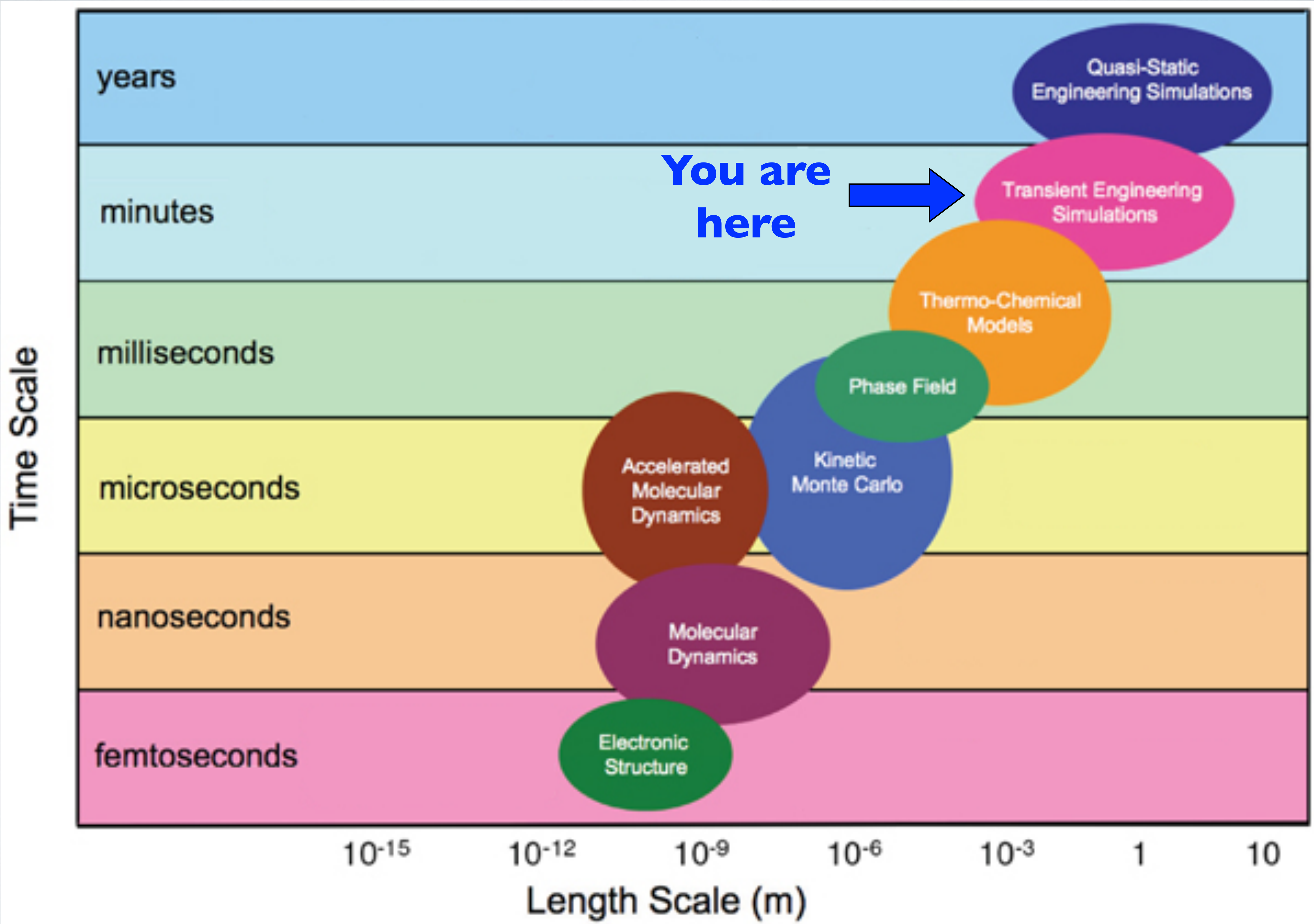
MODULE 3:
FINITE ELEMENT METHOD

Principles and Theory



http://www.lbl.gov/CS/html/exascale4energy/nuclear.html

I. Introduction

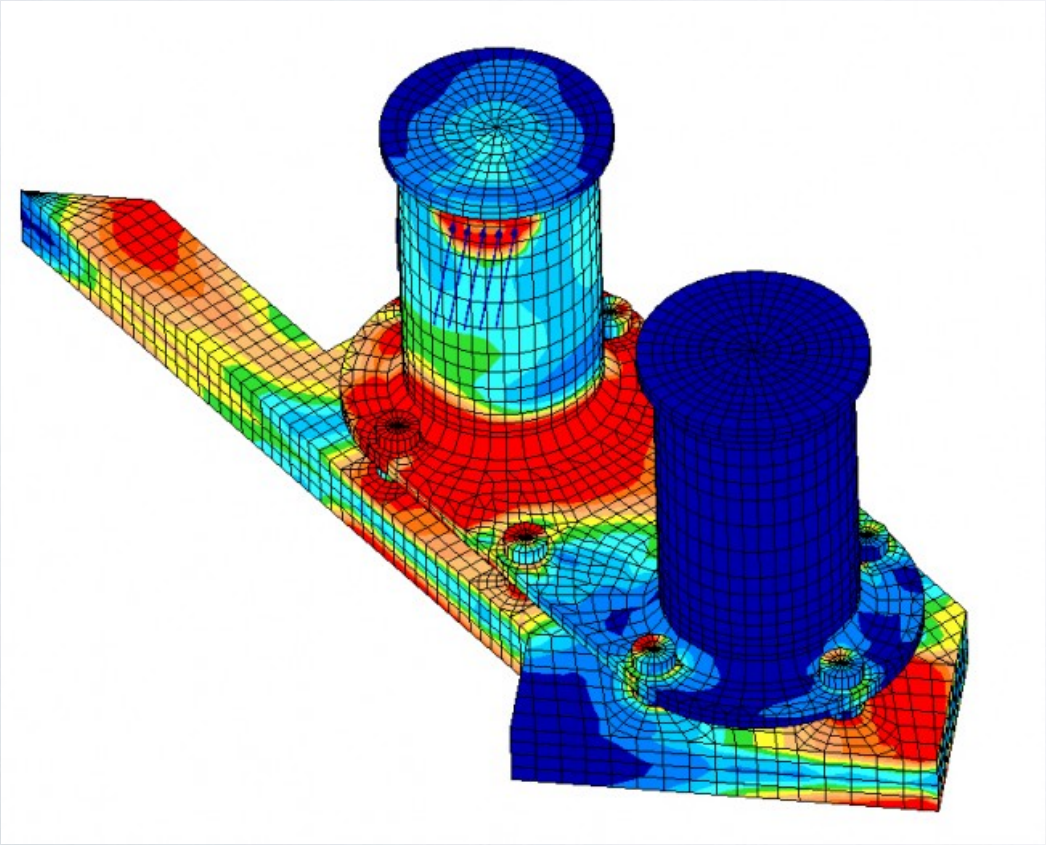
What is the finite element method?

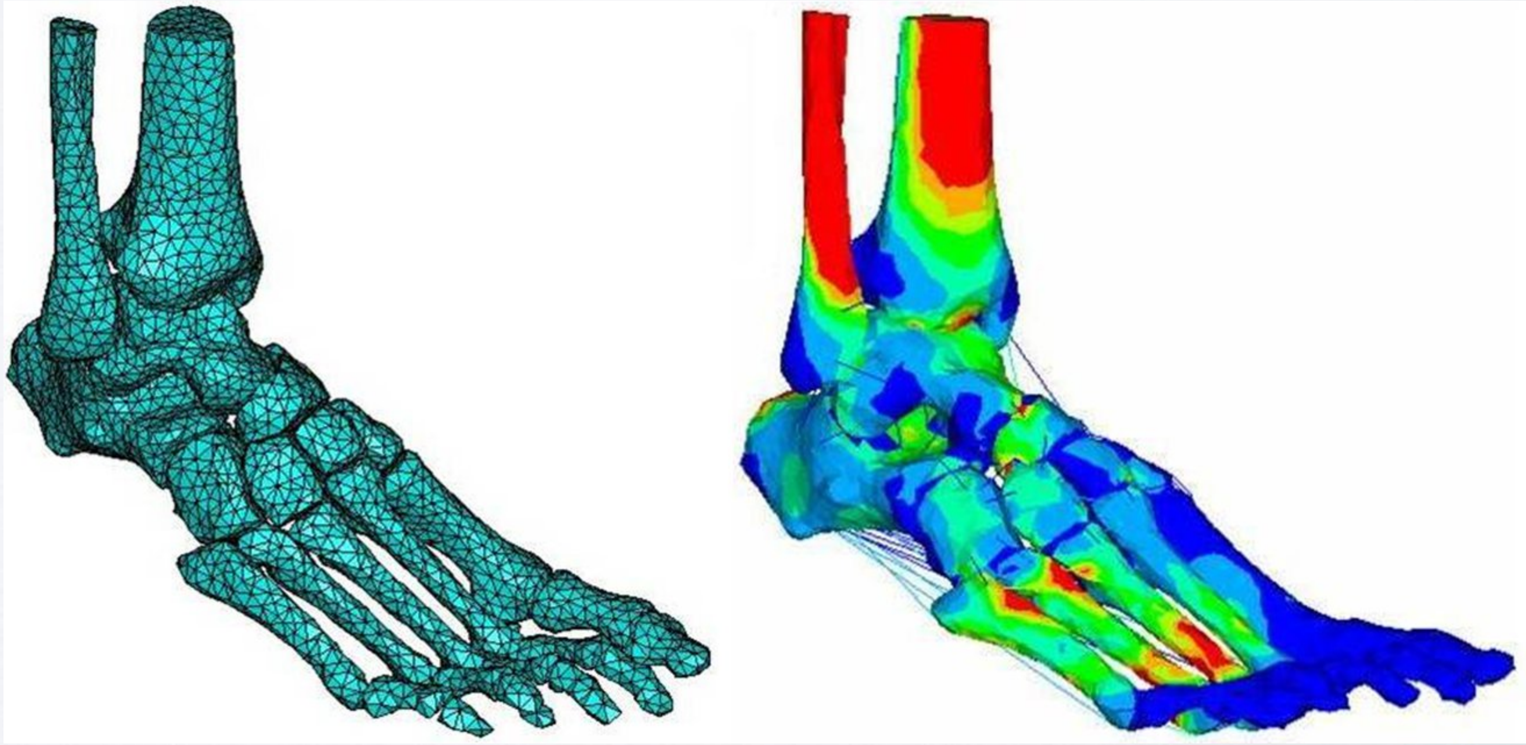
- FEM is a numerical method to solve **boundary value field problems** (i.e. PDEs with boundary conditions)

- For example, the heat equation over a finite domain with specified boundary conditions:

heat eqn $$\frac{\partial u}{\partial t} = \alpha \nabla^2 u$$

force balance $$\nabla \cdot \ddot{\sigma} = 0$$



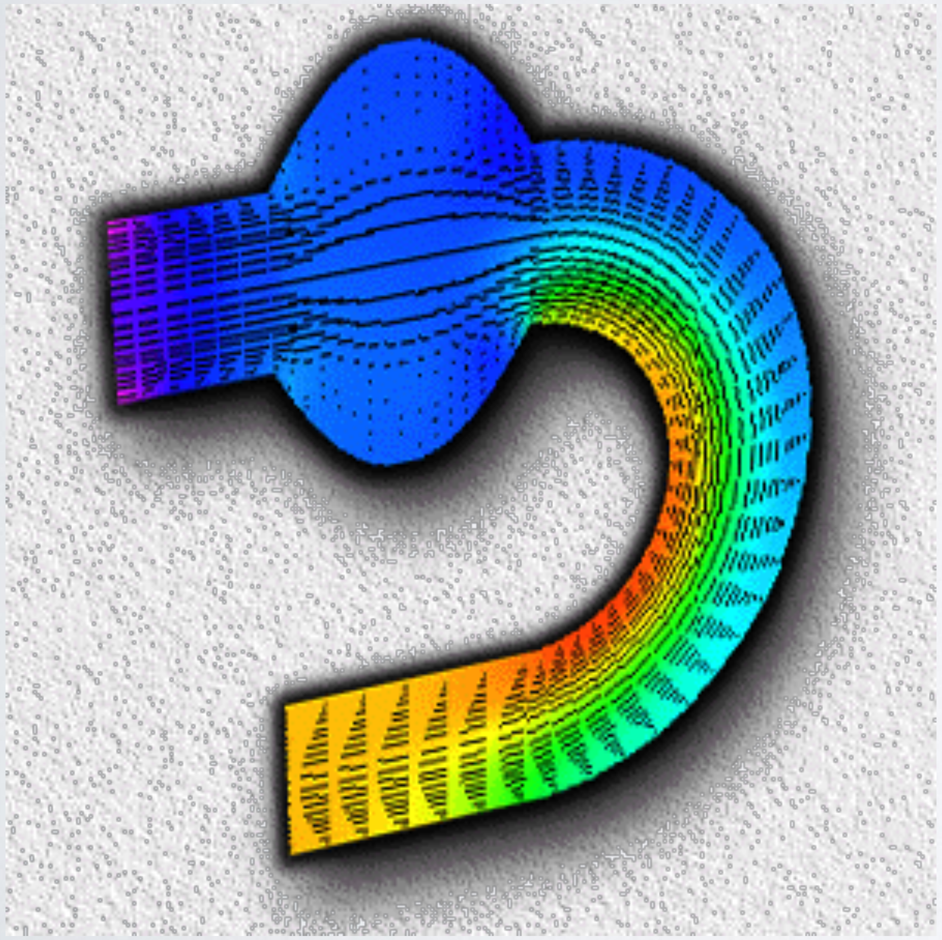


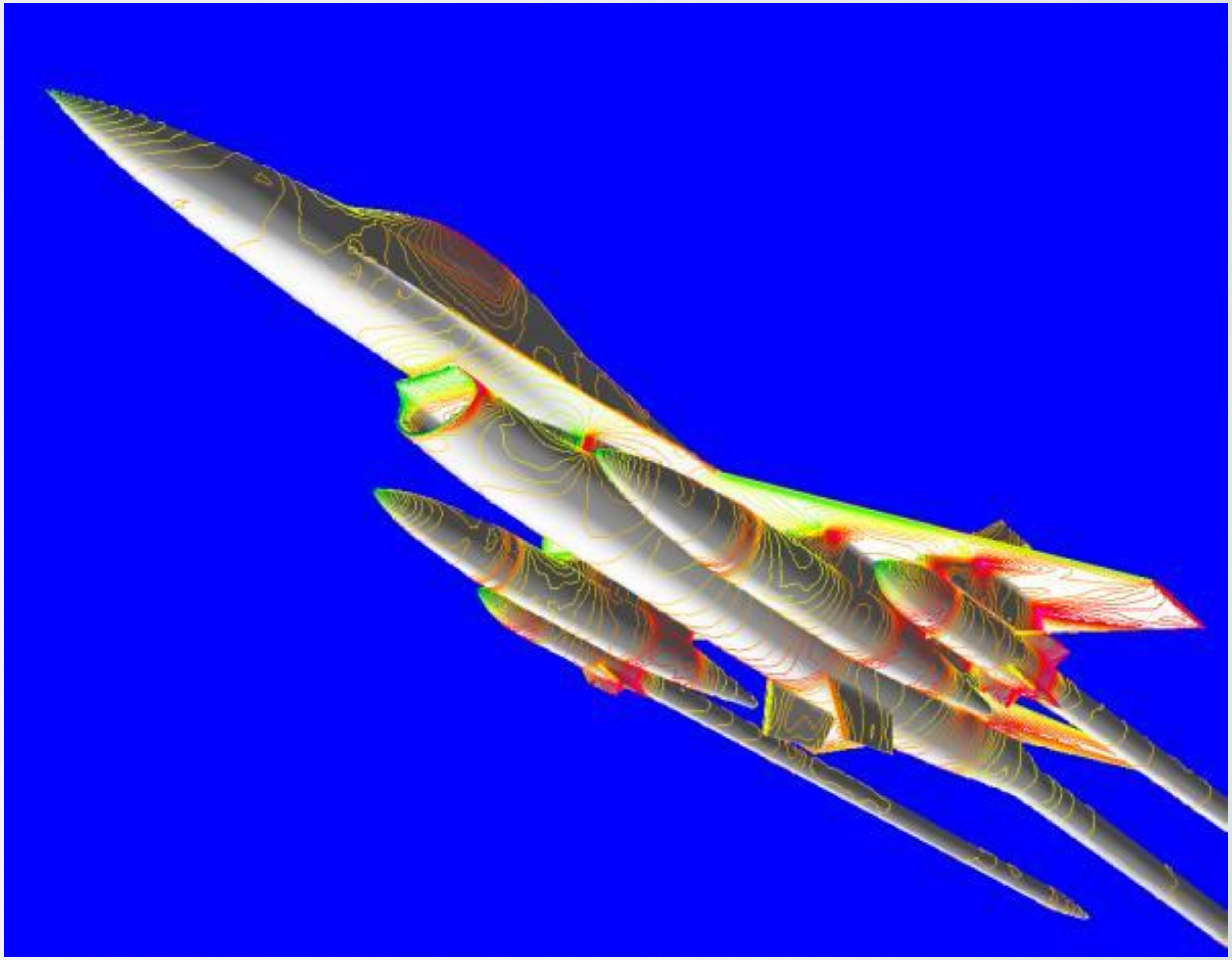
http://www.archonengineering.com/projects/finite-element-analysis/42/ http://imtronics.cereteth.gr/?p=528

What is the finite element method?

Navier-Stokes eqn

$$\rho\left(\frac{\partial\vec{v}}{\partial t}+\vec{v}\cdot\nabla\vec{v}\right)=-\nabla p+\mu\nabla^2\vec{v}+\vec{f}$$



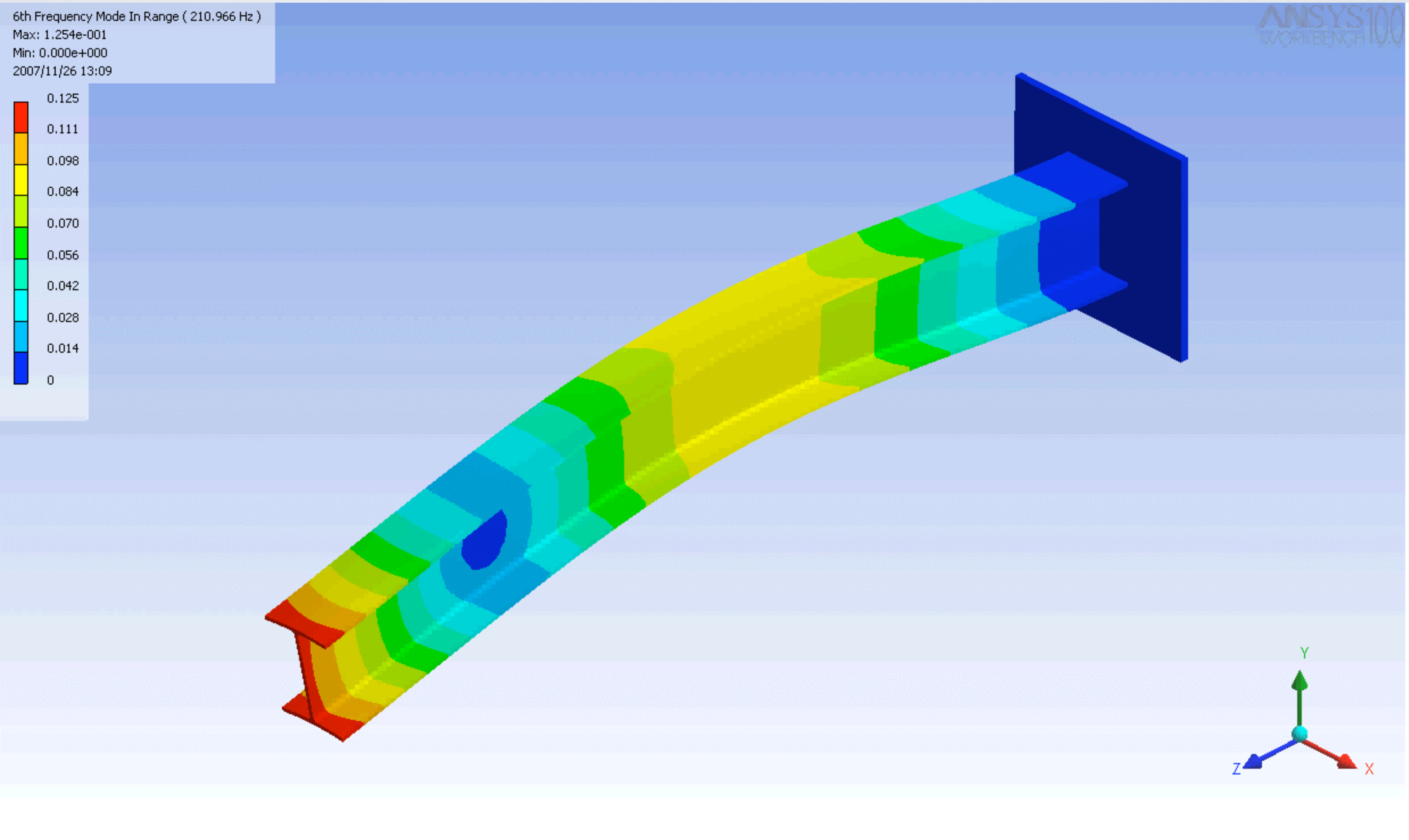


http://tetruss.larc.nasa.gov/apps/f16.html   http://www.diffpack.com/products/applications/app_main.html

What is the finite element method?

Euler-Bernoulli beam eqn

$$\frac{\partial^2}{\partial x^2}\left(EI\frac{\partial^2 w}{\partial x^2}\right) = -\mu\frac{\partial^2 w}{\partial t^2} + q(x)$$



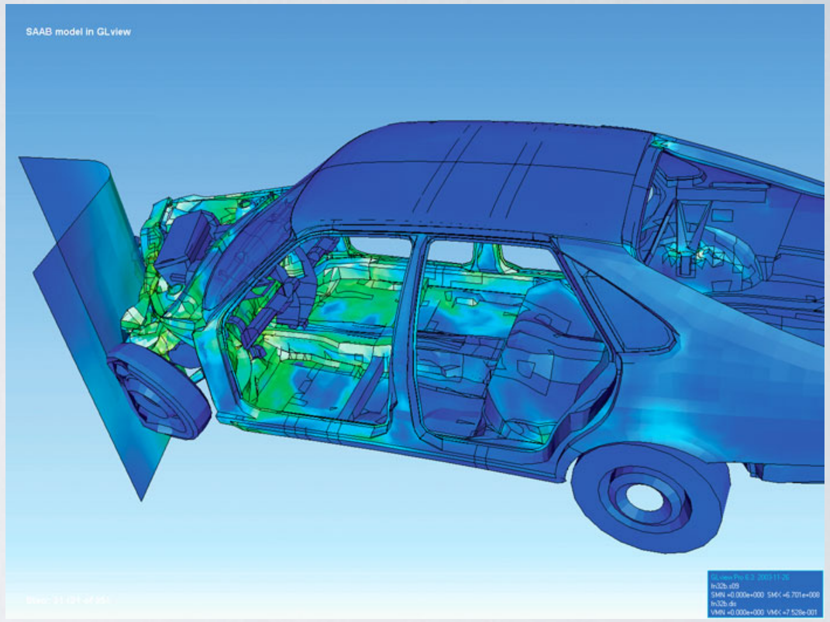
http://en.wikipedia.org/wiki/File:Beam_mode_6.gif

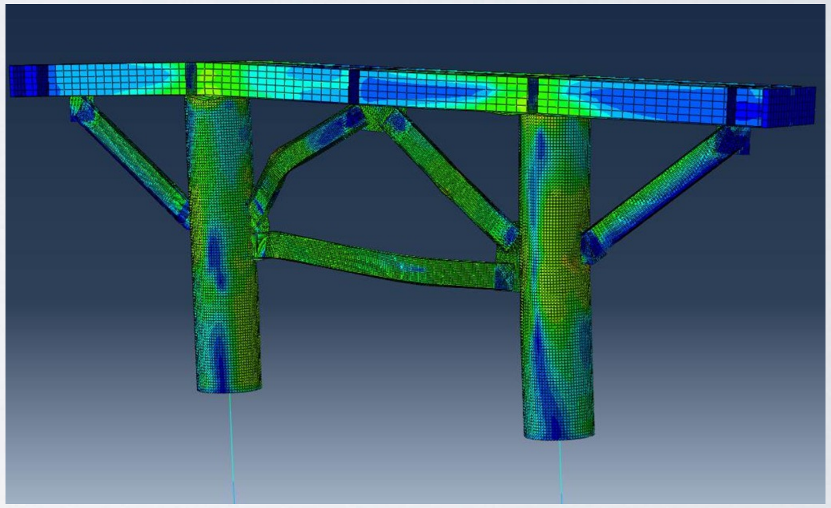
Why is it useful?

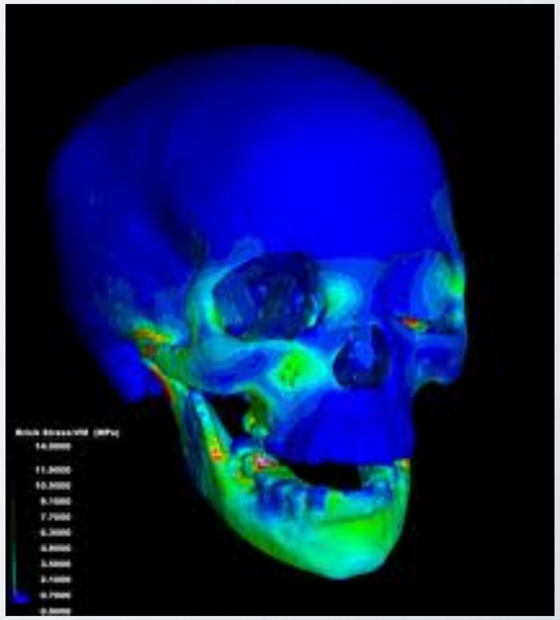
- Solves PDEs over **complex domains with spatio-temporally varying properties**
- Analytical theory cannot easily resolve complex details
- Intermediate between continuum and molecular methods
- Used to **predict and understand** materials properties and behaviors under different conditions
- Invaluable tool in equipment design, materials selection, and reliability assessment
- Extremely general and powerful methodology

What is it used for?

- Structural modeling
  - stress fields, deformations, heat fluxes, weakness identification
- Fluid mechanics
  - flow fields, plant design, microfluidics
- Electrostatics
  - charge distribution, electrostatic forces
- Biomechanics
  - skeletal analysis, prosthetic design & modeling, dentistry
- Reliability assessment & structural forensics
  - stress testing, failure analysis







http://www.engenya.com/the-finite-element-method-fem/ http://compbiomechblog.blogspot.com/2010/06/blog-post_20.html http://www.ce.ncsu.edu/news/article/21550/making-bridges-more-robust-to-earthquakes?from=rss

Is it used in industry?

- **YES!**

- Indispensable, standard tool in modern engineering design

- Massive cost savings in engineering design:
  - reduced labor, time & cost intensive experimentation
  - reliability assessment and failure prediction
  - identification of "soft spots" and reinforcement needs

- Structural design and optimization of complex structures can be performed in a matter of hours instead of months!*

- Reported ROI of 3:1 to 9:1 with investments of $5-20M

*Not so for de novo *materials* design

http://books.nap.edu/catalog.php?record_id=12199

II. Basic Principles

The fundamental idea

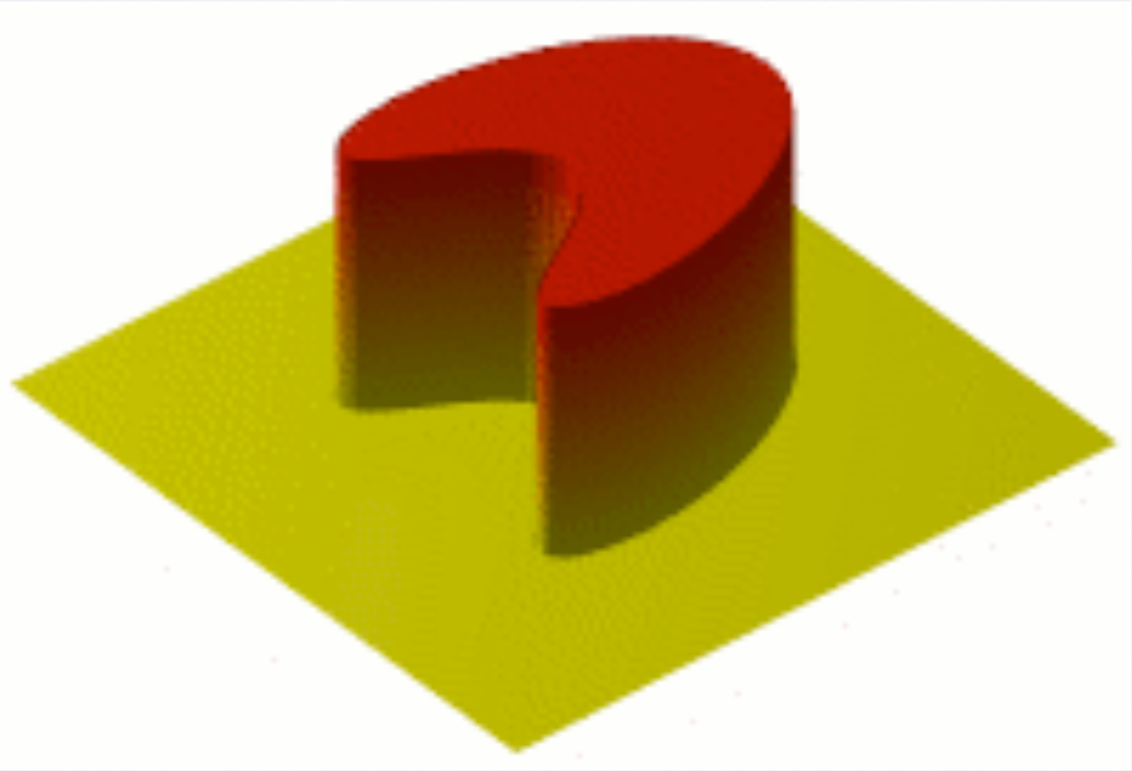
- **"Divide and conquer"**
  - recast continuum problem (infinite dimensional) into a finite dimensional problem by spatially partitioning domain
  - find local solutions within subdomains and patch together into approximate numerical solution

1. Split continuum into finite subdomains	meshing
2. Assign properties to each cell	properties
3. Choose basis set	basis
4. Formulate & solve coupled equations	solving

The fundamental idea

- For **steady state** solutions, we solve a set of coupled algebraic equations over the elements (linear algebra)

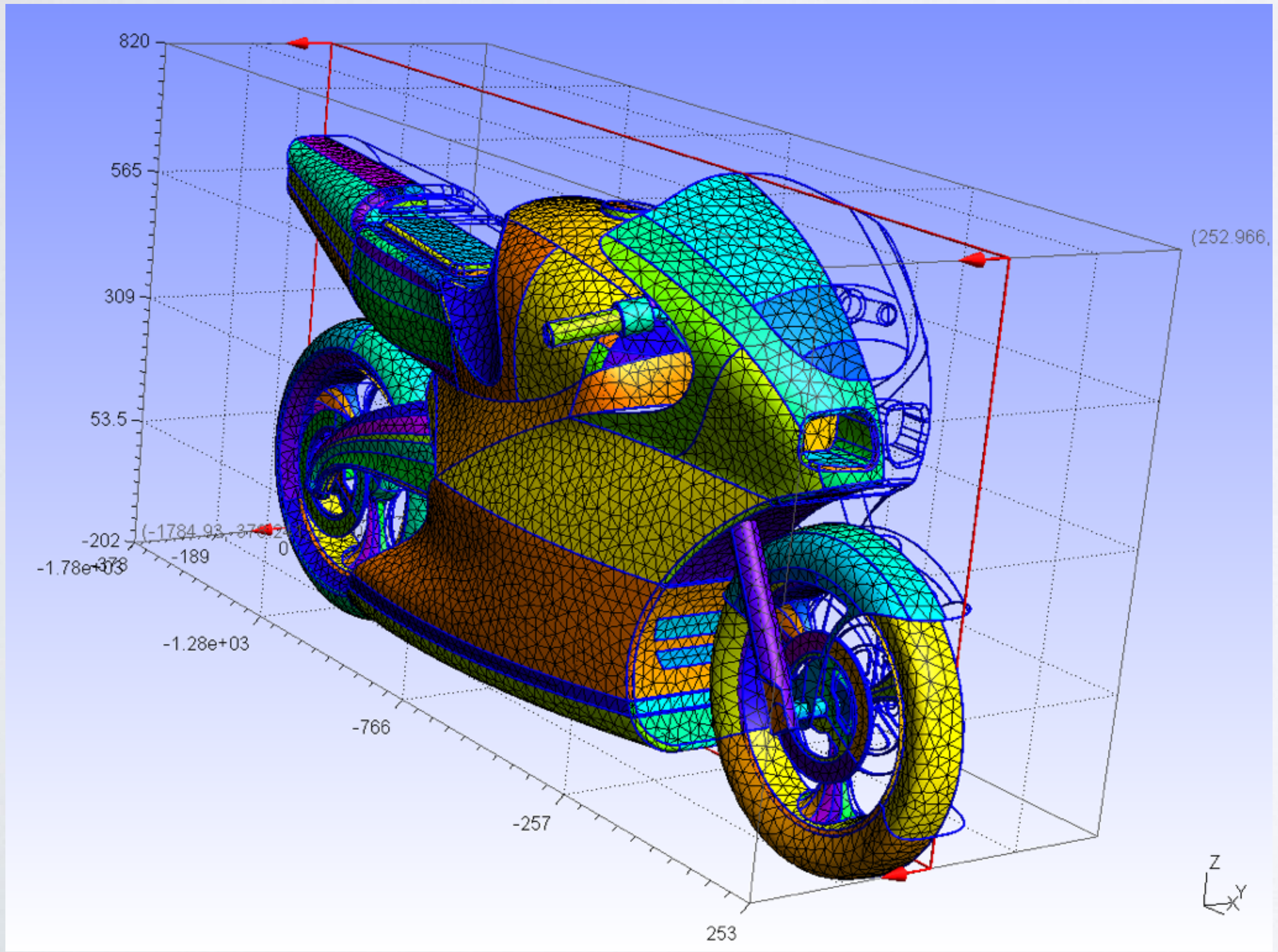
- For **time dependent** solutions, we solve a set of coupled ODEs over the elements (numerical integration)

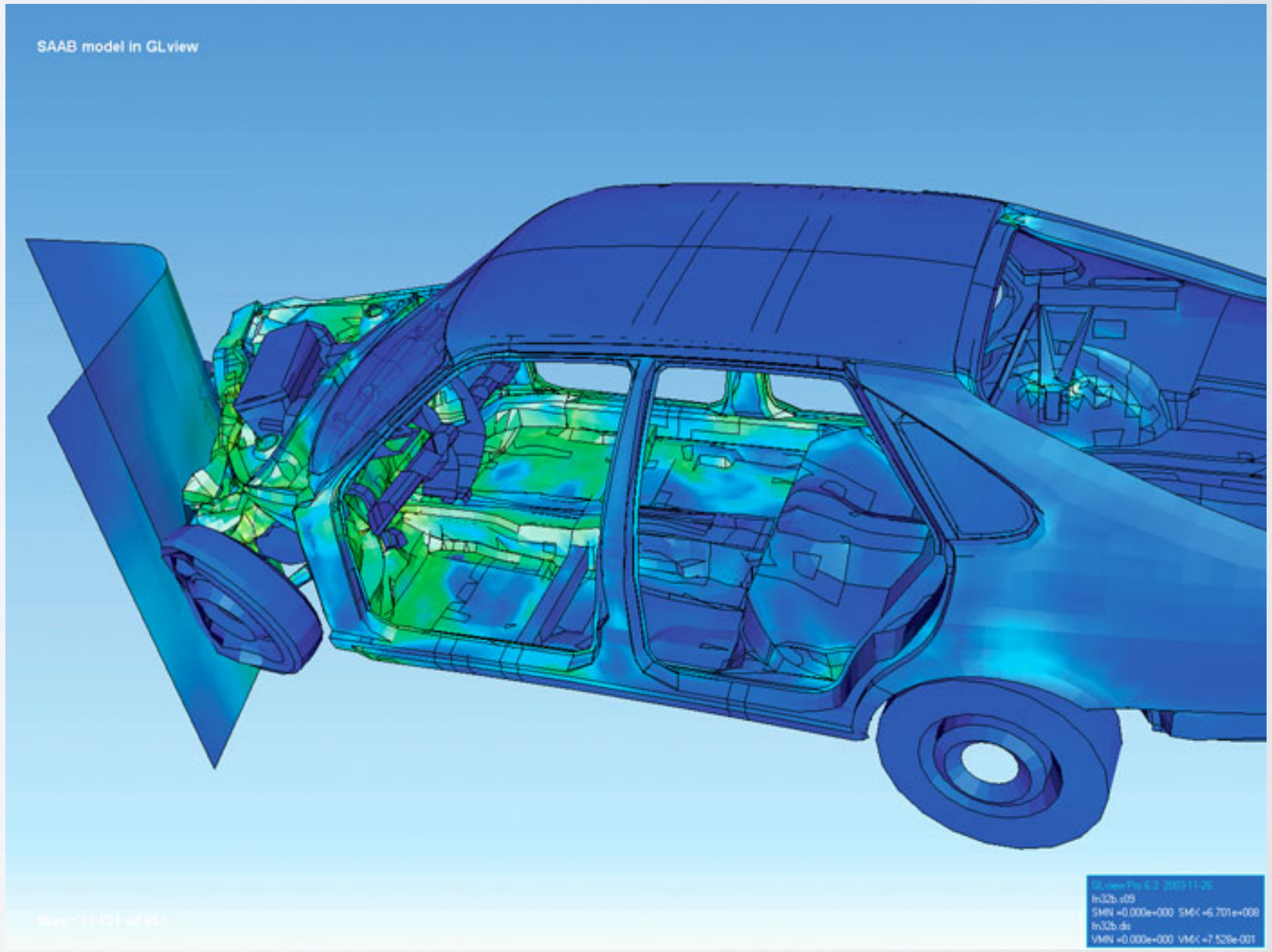


http://en.wikipedia.org/wiki/File:Heat_eqn.gif

Meshing

- Meshing is flexible, conformal, dynamic, and adaptive
  - fit geometry of interest
  - place more elements where solution expected to change most rapidly, or where detail is required
  - mesh can evolve with domain in time





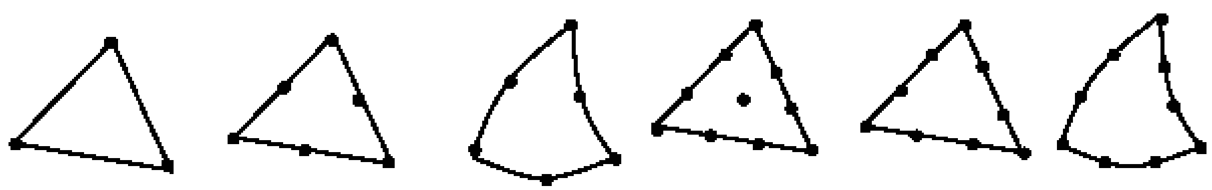
http://en.wikipedia.org/wiki/File:FAE_visualization.jpg http://geuz.org/gmsh/

Meshing

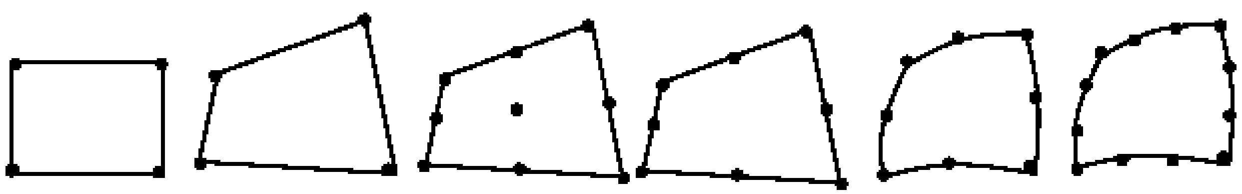
i) One-dimensional Elements

linear quadratic cubic

ii) Two-dimensional Elements

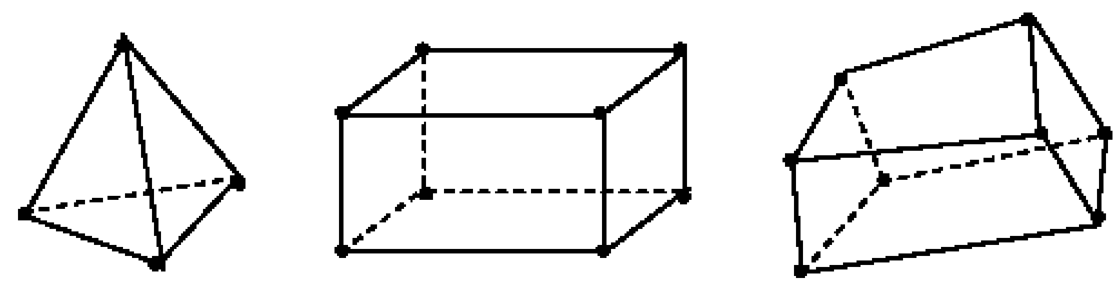


linear triangular | quadratic triangular | cubic triangular



Linear Rectangle | linear quadrilateral | quadratic quadrilateral | cubic quadrilateral

iii) Three-dimensional Elements



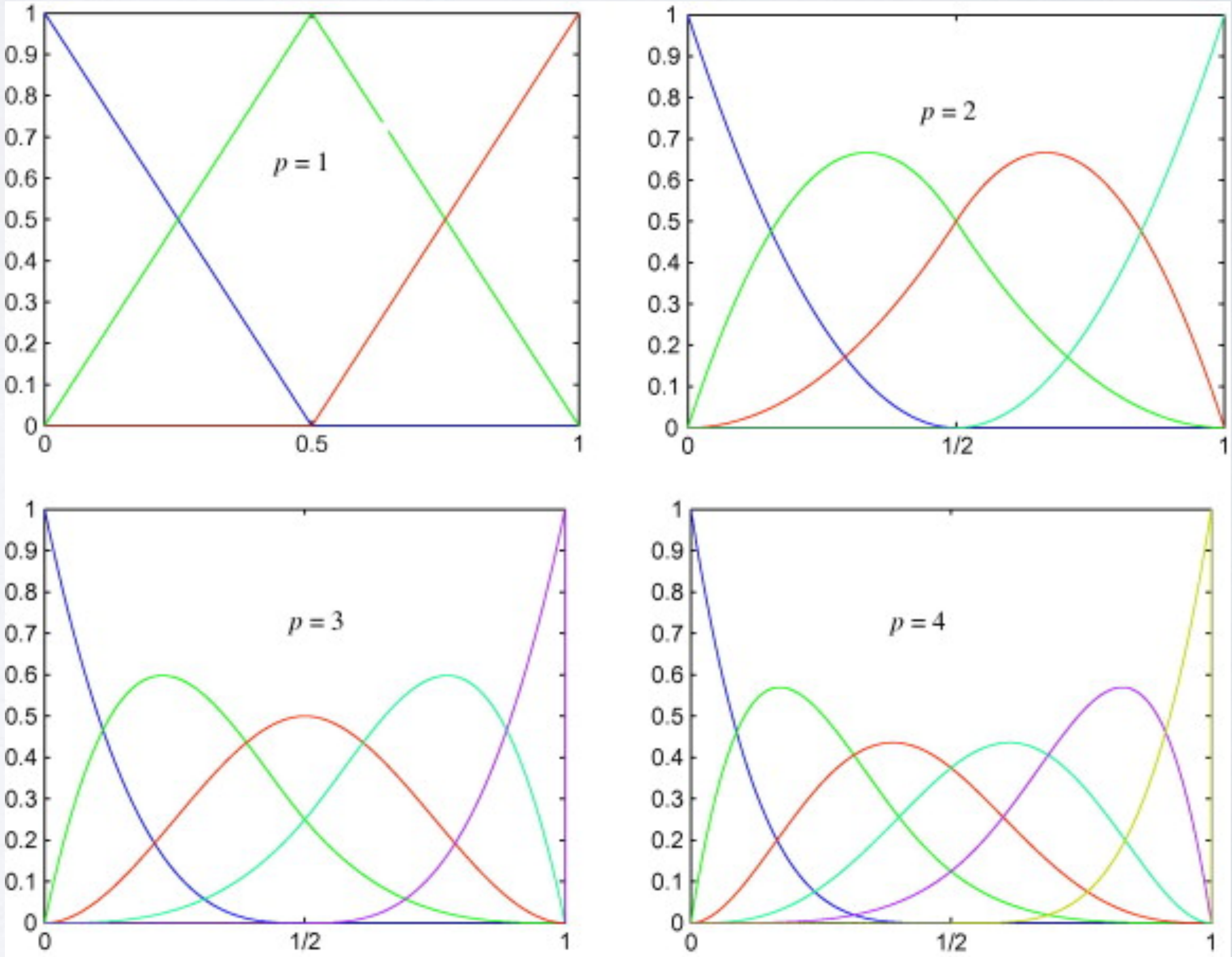
Tetrahedron | Right Prism | Hexahedron

Element types depend on the followings:

- Shape (1-D, 2-D, 3-D, triangular, quadrilateral, tetrahedron, etc.)
- Number and type of nodes (3-node, 4-node, etc.)
- Type of nodal variables ($\phi, \frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y}$, etc.)
- Type of interpolation functions

Basis functions

- Trial function is composed from **basis functions** defined within mesh elements
- Typically **compactly supported** fostering sparse matrix solutions and fast solvers (cf. spectral methods)
- Choice of basis function order dictated by rqmts of PDE (differentiability) and solution (smoothness)



1D B-spline bases of orders p=1-4

http://www.sciencedirect.com/science/article/pii/S1359836813001005

Weak solution

- Mathematically, FEM is a **Galerkin method**

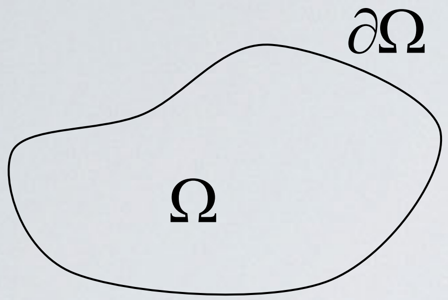
- Formulate a **weak solution** to the governing PDE, and fit trial functions to minimize the solution error

$$\nabla^2 \rho = f \xrightarrow[\text{weak formulation}]{} \int_\Omega \left(\nabla^2 \rho\right) v d\Omega = \int_\Omega f v d\Omega$$

- The RHS should hold for all trial functions, **v**, which are linear combinations of basis functions

- In this sense the formulation is **weak**, since the solution ρ does not hold *absolutely*, just for *all trial functions* **v**

General steps



$$\mathcal{L}u(\vec{r}) = f(\vec{r})$$

continuum problem

$$\hat{u}(\vec{r}) = \sum_{k=1}^{n} c_k \phi_k(\vec{r})$$

trial function = linear combination of basis functions

$$\mathbf{L}\underline{\hat{\mathrm{u}}} = \underline{\mathrm{f}}$$

$$L_{ij} = \int_\Omega \phi_i \left(\mathcal{L}\phi_j\right) d\Omega$$

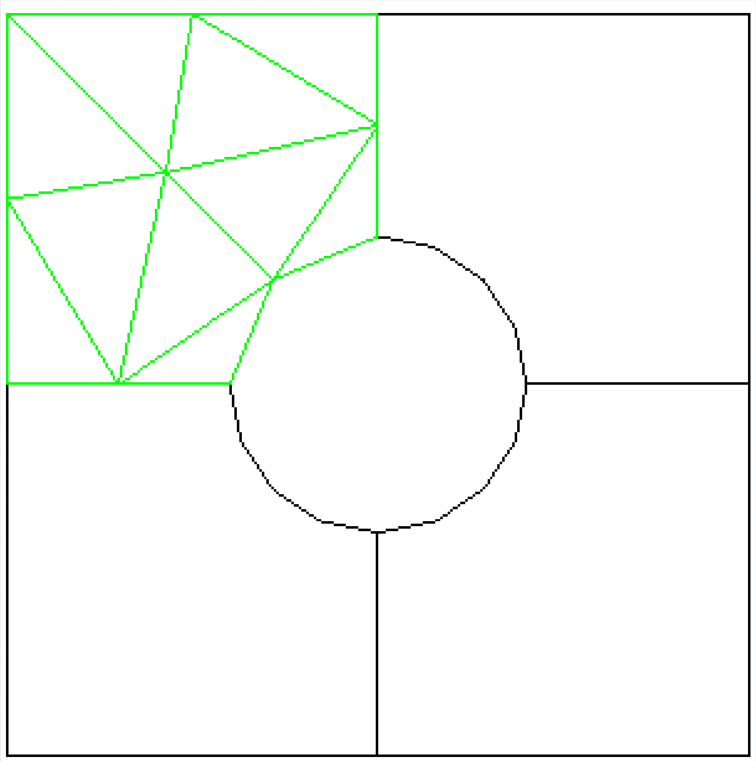
$$f_i = \int_\Omega \phi_i f \, d\Omega$$

Galerkin variational solution

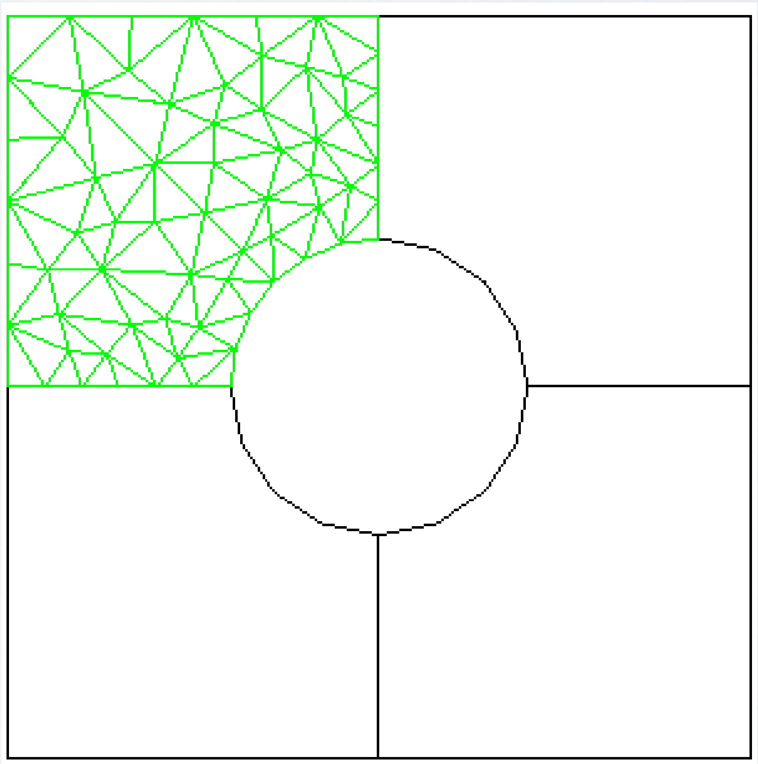
Error sources

- Residual errors from:
  - domain discretization
  - choice of basis
  - formulation errors
  - numerical solution

1. Domain discretization



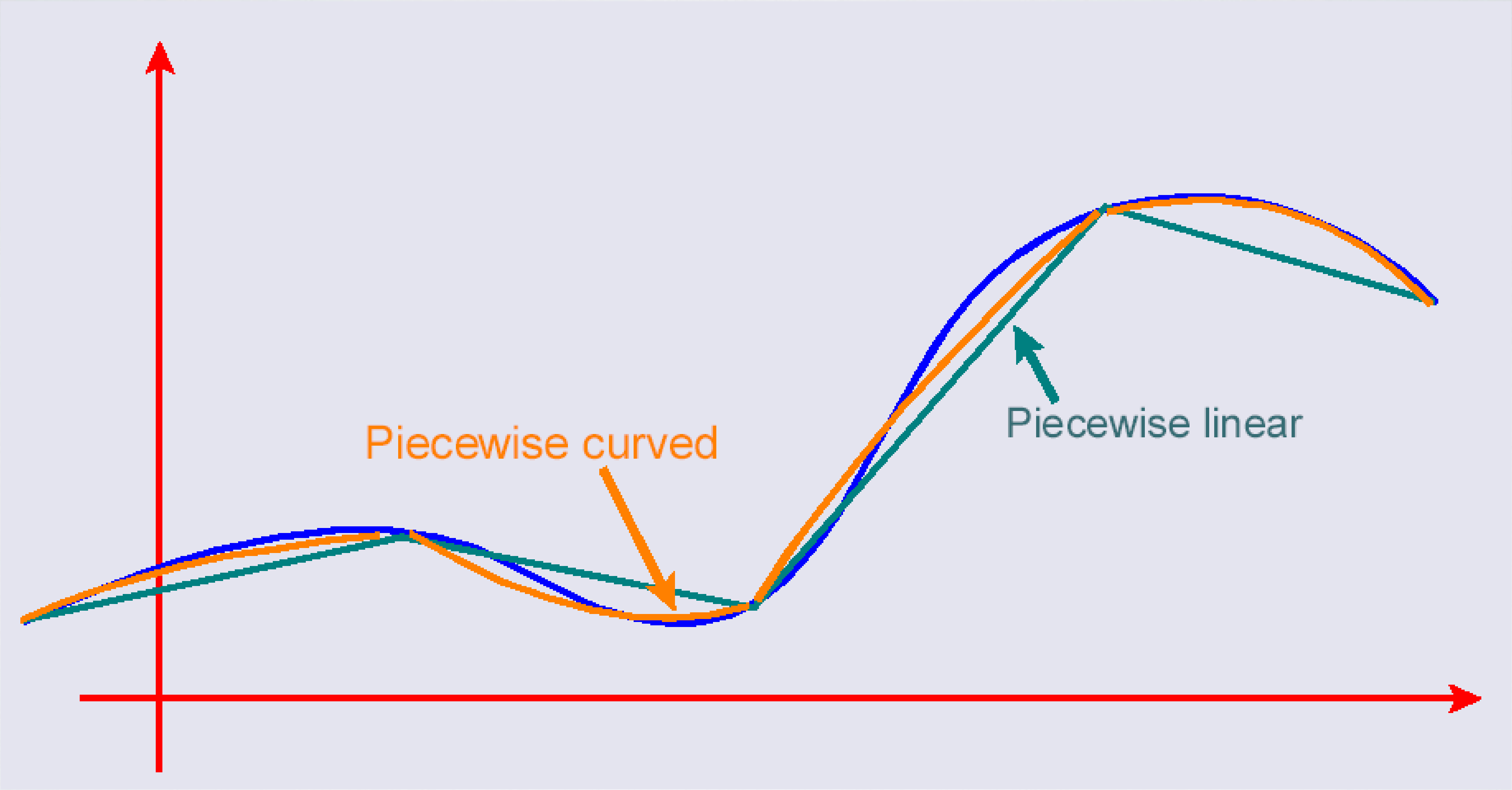
Discretization error due to poor geometry representation.



Discretization error effectively eliminated.

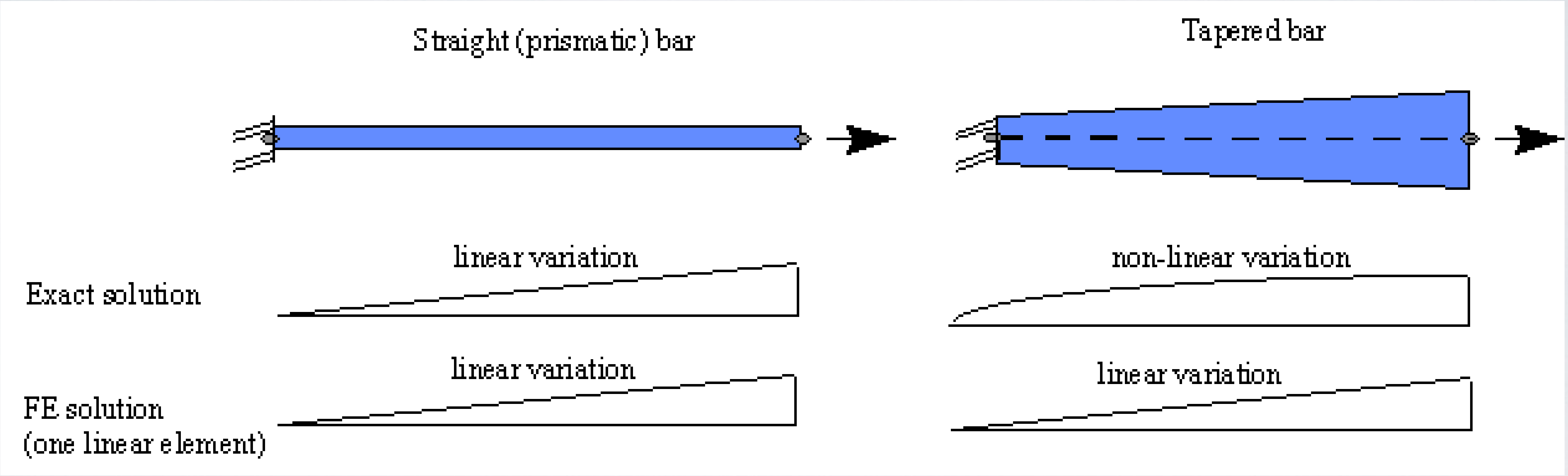
Error sources

II. Basis set



Error sources

III. Formulation



Adaptive FEM

- Error estimation can quantify the error in the numerical approximation relative to the continuum solution

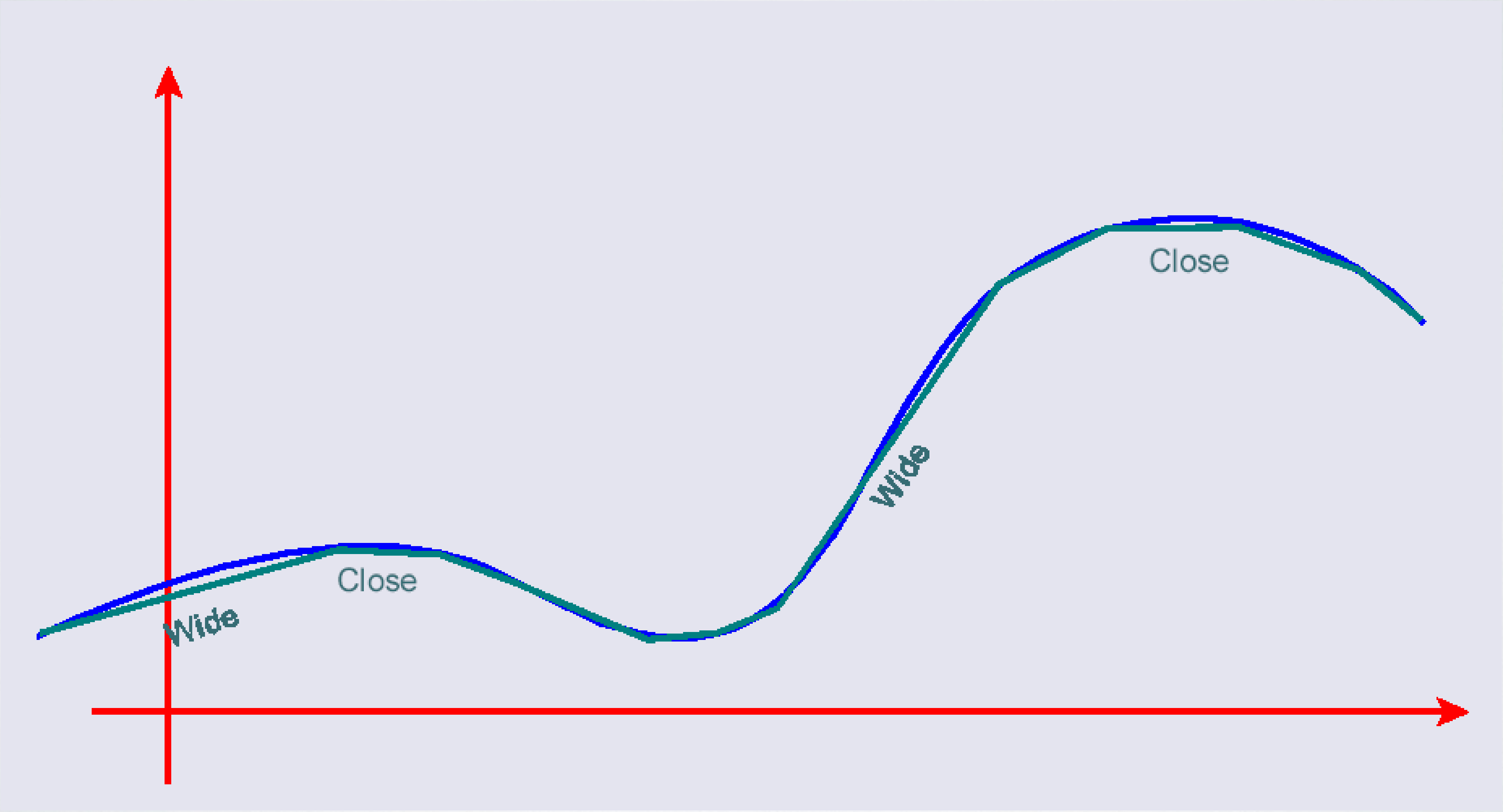
- Adaptive mesh optimization can refine the discretization to reduce the error to within a user specified tolerance:

  - r-adaptivity - moving nodes
  - h-adaptivity - element refinement / unrefinement
  - p-adaptivity - basis function order modification

- Combinations are possible: hpr-refinement

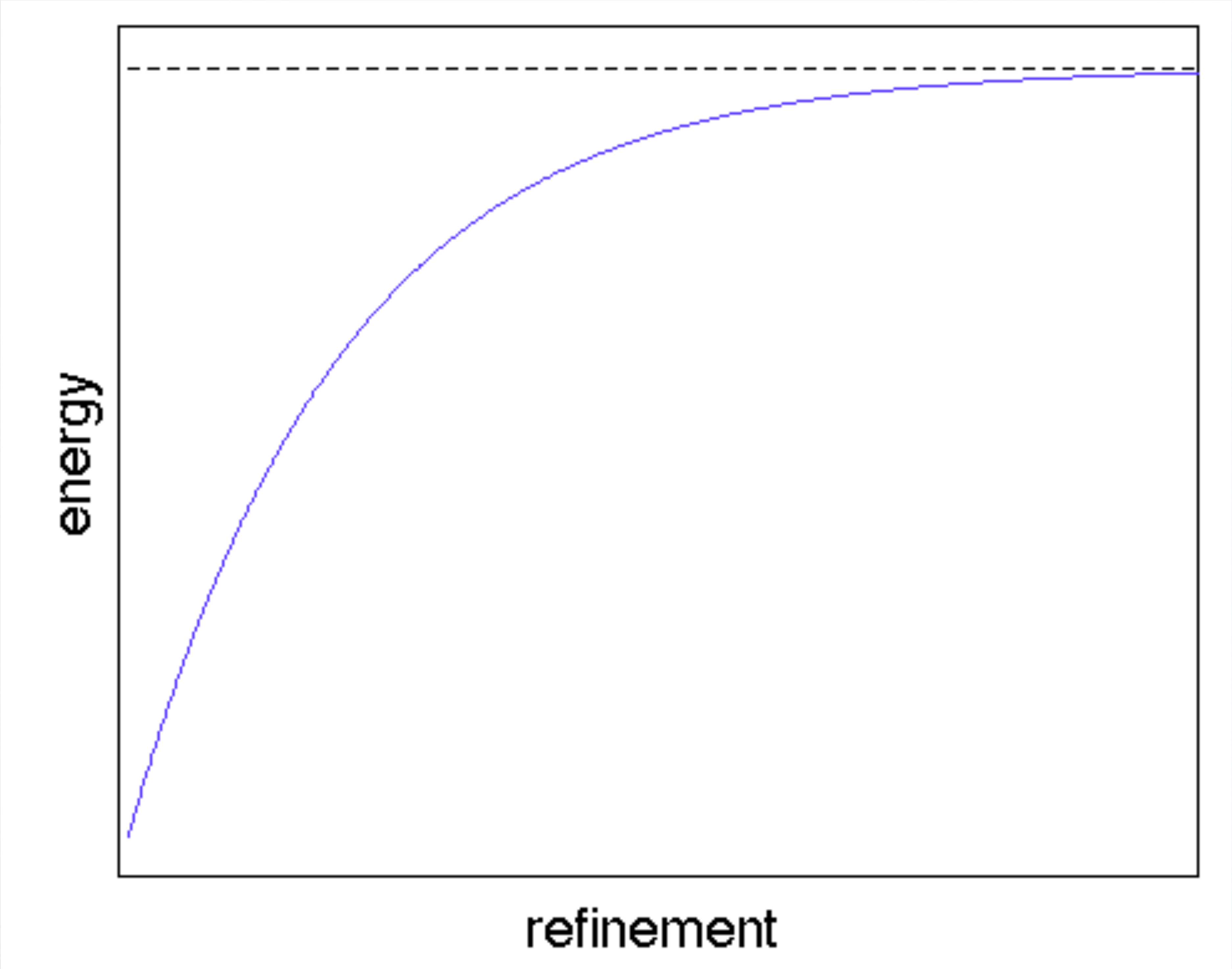
Adaptive FEM

- hr-adaptivity:
  finer discretization at rapidly changing domain regions



Convergence

- Internal check of convergence that solution converges with increasing refinement / discretization



Limitations and Caveats

- Approximate solution with inherent errors
- No closed form solution generated
- Substantial experience / judgement required to synthesize good model
- Computationally expensive
- Data intensive I/O and computation

III. Simple Example

FEM of 1D steady-state heat equation

$$\frac{\partial u}{\partial t} = \alpha \nabla^2 u + \frac{1}{\rho C_p} q$$ const props

$$\Rightarrow \quad \nabla^2 u + \frac{1}{\alpha \rho C_p} q = 0$$ steady state

$$\Rightarrow \quad \nabla^2 u + \frac{1}{k} q = 0$$

$$\Rightarrow \quad \boxed{\frac{d^2 u}{dx^2} + \frac{1}{k} q(x) = 0}$$ 1D

temperature $[u] = K$

thermal diffusivity $[\alpha] = \dfrac{m^2}{s}$

heat capacity $[C_p] = \dfrac{J}{kg.K}$

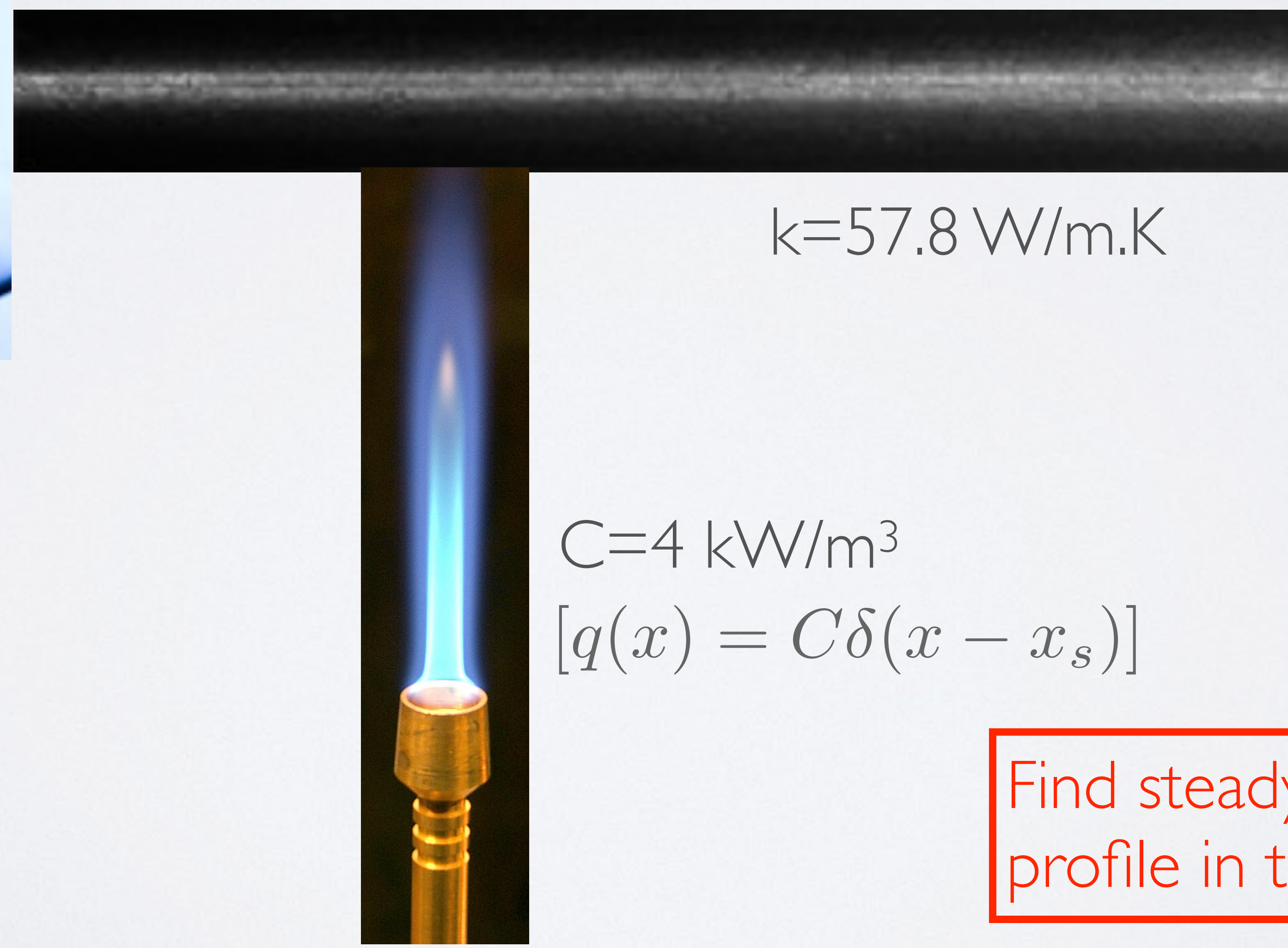
density $[\rho] = \dfrac{kg}{m^3}$

volumetric source $[q] = \dfrac{W}{m^3}$

thermal conductivity $[k] = \dfrac{W}{m.K}$

System

x=0m x_S=0.4m x=1m



k=57.8 W/m.K

T=0°C

T=0°C

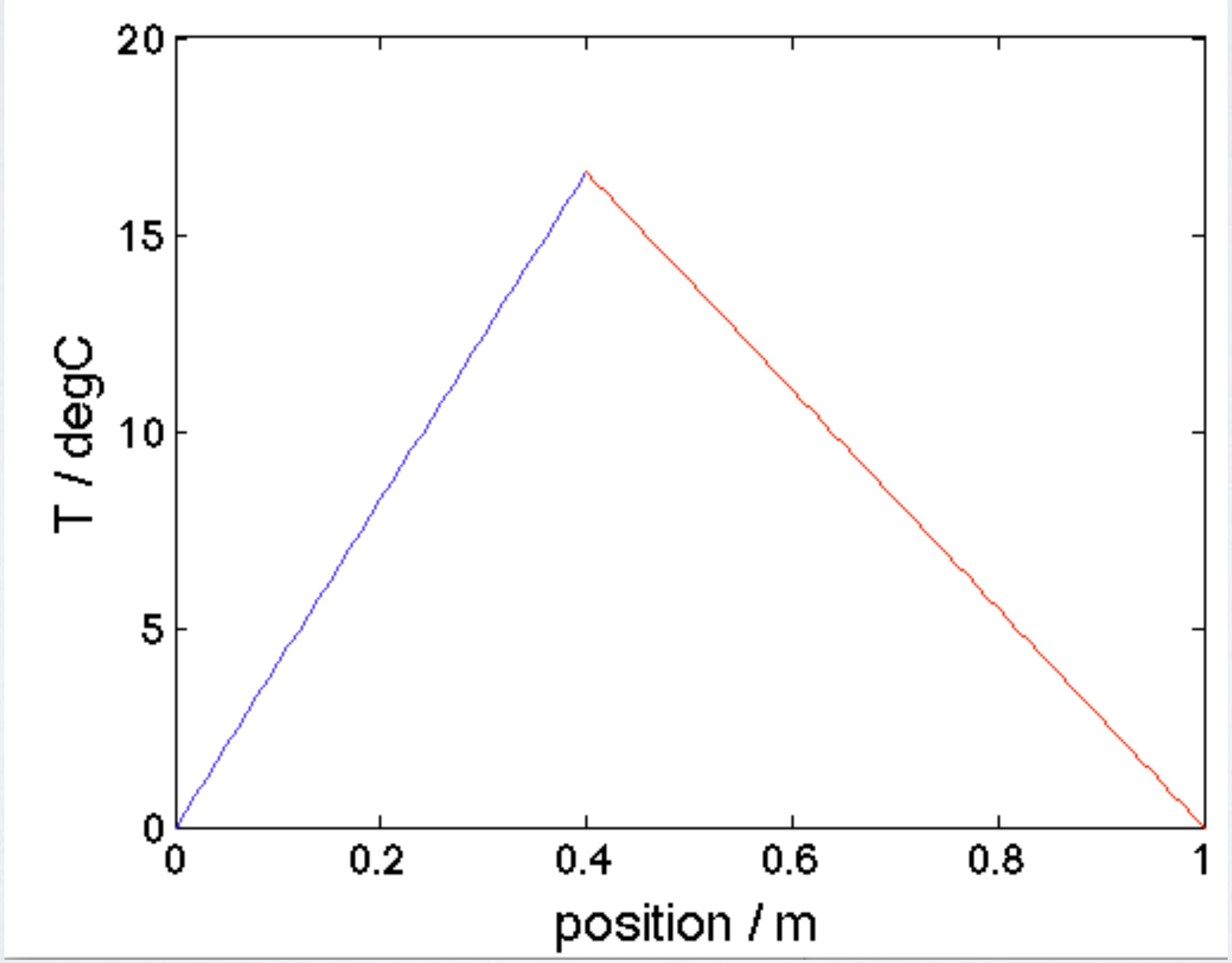
C=4 kW/m^3

$$[q(x) = C\delta(x - x_s)]$$

Find steady-state temperature profile in the iron bar, u(x)

Analytical solution

$$u(x) = \begin{cases} \frac{C}{k}(1-x_s)x, & 0 \le x \le x_s \\ \frac{C}{k}x_s(1-x), & x_s \le x \le 1 \end{cases}$$



I. Meshing

$$x_0 = 0 < x_1 < x_2 < \ldots < x_n < x_{n=1} = 1$$

$$\Delta x = x_{j+1} - x_j = \text{const.}$$

II. Element properties

- All elements identical size and thermal conductivity, k

III. Basis set

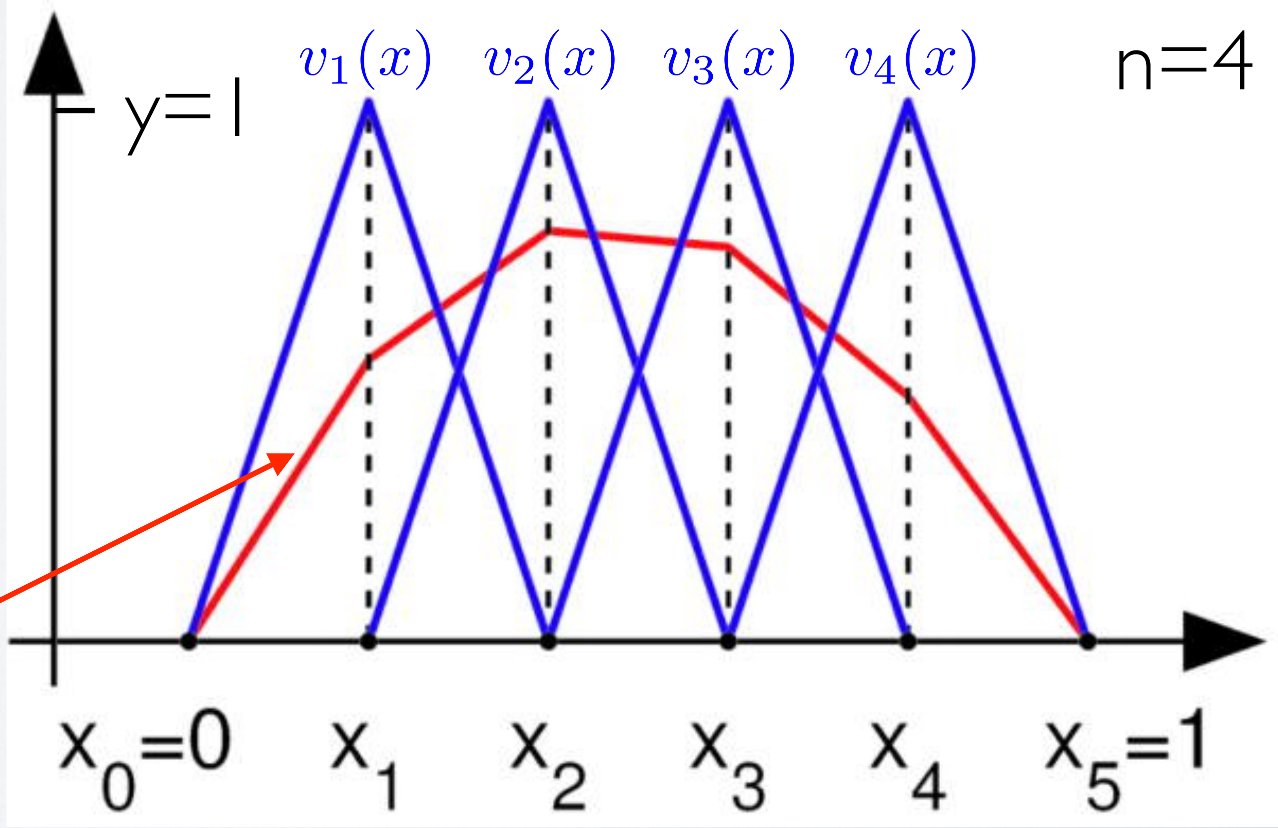
- Simplest choice: **"tent functions"**
  - one-dimensional linear interpolants with compact support

$$v_k(x) = \begin{cases} \frac{x - x_{k-1}}{x_k - x_{k-1}}, & \text{for } \; x_{k-1} \le x < x_k \\ \frac{x_{k+1} - x}{x_{k+1} - x_k}, & \text{for } \; x_k \le x < x_{k+1} \\ 0, & \text{otherwise} \end{cases}$$

$$v_k'(x) = \begin{cases} \frac{1}{x_k - x_{k-1}}, & \text{for } \; x_{k-1} \le x < x_k \\ -\frac{1}{x_{k+1} - x_k}, & \text{for } \; x_k \le x < x_{k+1} \\ 0, & \text{otherwise} \end{cases}$$

- Appropriate choice for problem - expect linear soln

$$u(x) = \sum_{i=1}^{4} u_i v_i(x)$$



IV. Weak formulation

$$u''(x) = -\frac{C}{k}\delta(x - x_s)$$ 1D, steady state, const props, heat equation

$$\int_0^1 \left[-\frac{C}{k}\delta(x - x_s)\right] v(x)dx = \int_0^1 u''(x)v(x)dx$$ weak formulation*

$$= [u'(x)v(x)]_0^1 - \int_0^1 u'(x)v'(x)dx$$

by parts

$$= -\int_0^1 u'(x)v'(x)dx$$ v(0)=v(1)=0

*If u(x) satisfies for every smooth v(x) that satisfies BCs, then u(x) solves:

$$u''(x) = -\frac{C}{k}\delta(x - x_s)$$

$$u(0) = u(1) = 0$$

IV. Weak formulation

Exploiting finite support of each basis function:

$$\int_{x_{j-1}}^{x_{j+1}} \left[-\frac{C}{k}\delta(x - x_s)\right] v_j(x)dx = -\int_{x_{j-1}}^{x_{j+1}} u'(x)v_j'(x)dx$$

governing eqn in each element

Expanding solution in basis set:

$$u(x) = \sum_{i=1}^{n} u_i v_i(x) \qquad u'(x) = \sum_{i=1}^{n} u_i v_i'(x)$$

u_i are expansion coefficients

Inserting solution expressed in basis set:

$$\int_{x_{j-1}}^{x_{j+1}} \left[-\frac{C}{k}\delta(x - x_s)\right] v_j(x)dx = -\sum_{i=1}^{n} u_i \int_{x_{j-1}}^{x_{j+1}} v_i'(x)v_j'(x)dx$$

governing eqn in each element

IV. Matrix form

$$-\sum_{i=1}^{n} u_i \int_{x_{j-1}}^{x_{j+1}} v_i'(x)v_j'(x)dx = \int_{x_{j-1}}^{x_{j+1}} \left[-\frac{C}{k}\delta(x-x_s)\right] v_j(x)dx$$

governing eqn in each element

Finite dimensional basis admits simple matrix representation:

$$-\mathbf{L}\underline{\mathrm{u}} = \underline{\mathrm{b}}$$

where

$$L_{ij} = \int_{x_{j-1}}^{x_{j+1}} v_i'(x)v_j'(x)dx$$

"stiffness" matrix

$$b_j = -\frac{C}{k}\int_{x_{j-1}}^{x_{j+1}} \delta(x-x_s)v_j(x)dx$$

These matrix & vector elements can be explicitly evaluated!

IV. Matrix elements

Grinding through the (simple) algebra:

$$L_{ij} = \begin{cases} \frac{1}{x_j - x_{j-1}} + \frac{1}{x_{j+1} - x_j}, & \text{if } \; i = j \\ -\frac{1}{x_j - x_{j-1}}, & \text{if } \; i = (j-1) \\ -\frac{1}{x_{j+1} - x_j}, & \text{if } \; i = (j+1) \\ 0, & \text{otherwise} \end{cases}$$

compactly supported basis functions make L sparse

$$b_j = \begin{cases} -\frac{C}{k} \frac{x_s - x_{j-1}}{x_j - x_{j-1}}, & \text{for } j \text{ s.t. } x_{j-1} \leq x_s \leq x_j \\ -\frac{C}{k} \frac{x_{j+1} - x_s}{x_{j+1} - x_j}, & \text{for } j \text{ s.t. } x_j \leq x_s \leq x_{j+1} \\ 0, & \text{otherwise} \end{cases}$$

IV. Solve

- Stiffness matrix is sparse, symmetric, and positive definite
- Efficient solution via LU factorization or Cholesky decomposition
- In MATLAB: $\underline{\mathrm{u}} = -\mathbf{L} \backslash \underline{\mathrm{b}}$
- Recovering solution: $u(x) = \sum_{i=1}^{n} u_i v_i(x)$

u_i are expansion coefficients

General case - recover solution at arbitrary points x*:

$$x_p \leq x^* < x_{p+1}$$

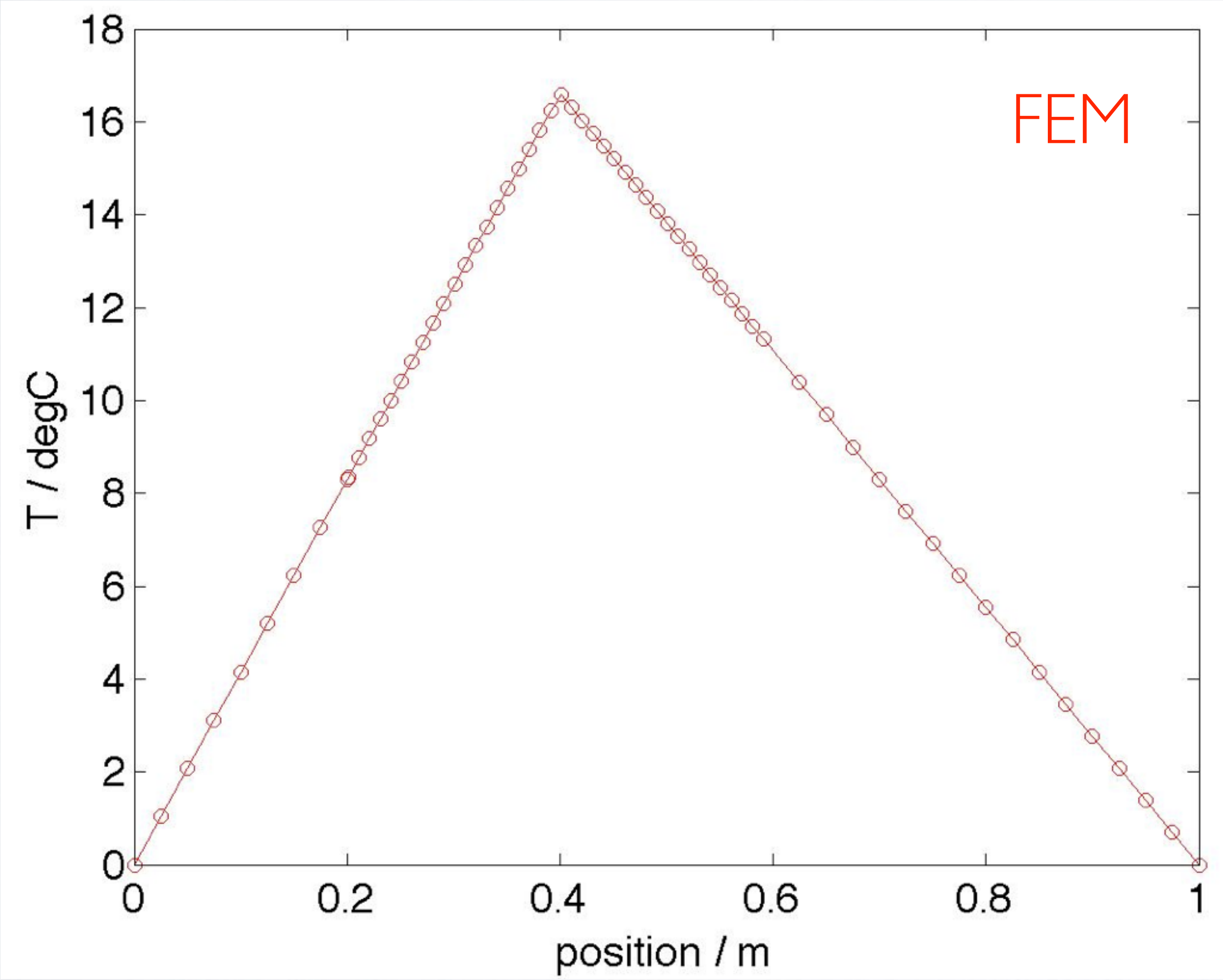
$$u(x^*) = u_p \left(\frac{x_{p+1} - x^*}{x_{p+1} - x_p} \right) + u_{p+1} \left(\frac{x^* - x_p}{x_{p+1} - x_p} \right)$$

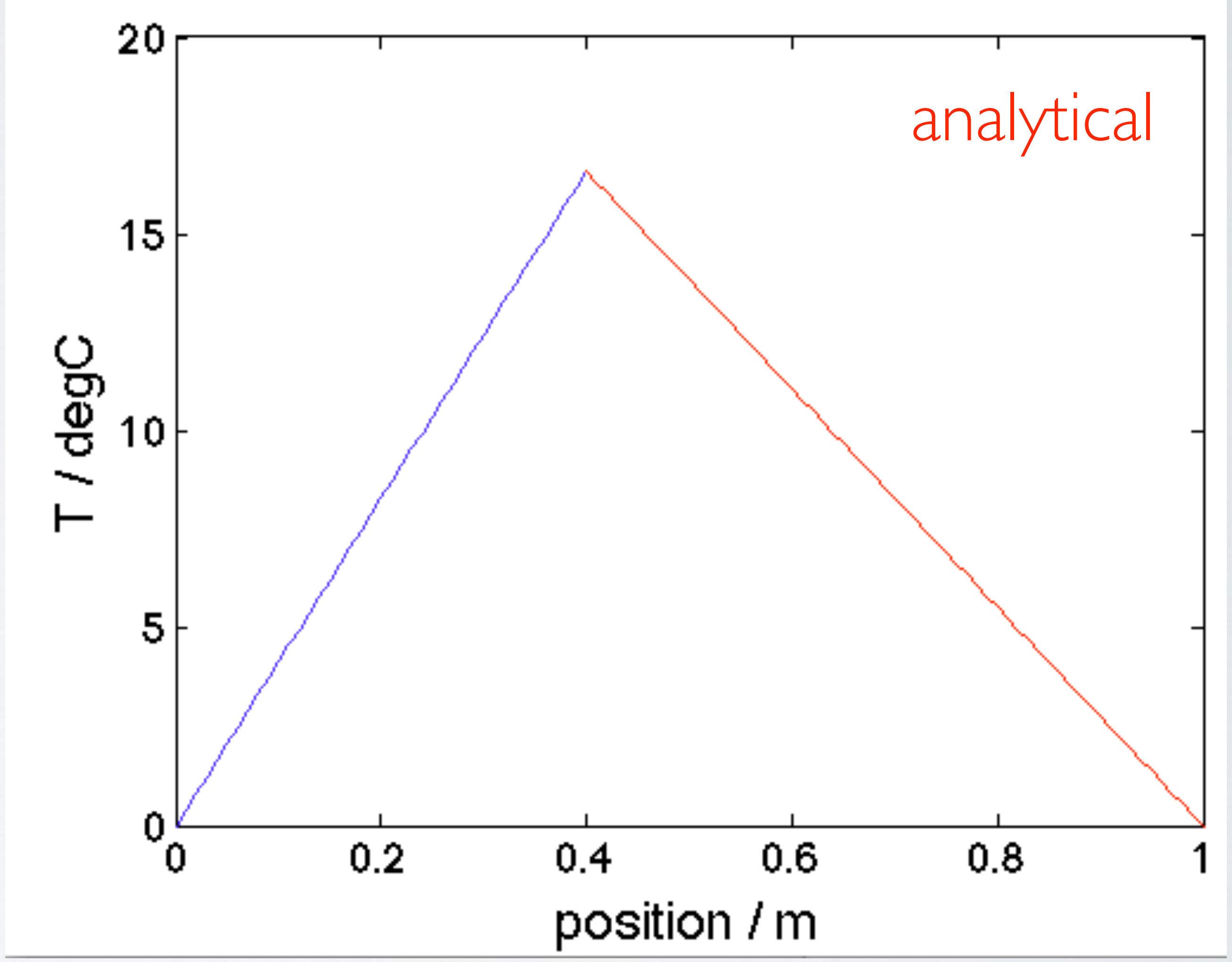
v_i are compactly supported, at most two are non-zero

Special case - recover solution only at grid points x_p:

$u(x_p) = u_p$ ← very simple - the solution **is** the expansion coefficients!

IV. Solve


FEM
T / degC
18
16
14
12
10
8
6
4
2
0
0
0.2
0.4
0.6
0.8
1
position / m


analytical
T / degC
20
15
10
5
0
0
0.2
0.4
0.6
0.8
1
position / m

IV. FEM Packages

FEM software

OOF2	NIST www.ctcms.nist.gov/oof/oof2	FREE
AUTODESK.	Autodesk Simulation Multiphysics www.autodesk.com	$4k
ANSYS	Ansys www.ansys.com	UIUC lic.
OOFEM.ORG	OOFEM www.oofem.org/en/oofem.html	FREE
Dynamic Finite Element Program Suite Impact	Impact http://impactprogram.wikispaces.com	FREE
Elmer	CSC www.csc.fi/english/pages/elmer	FREE
SIMULIA	Dassault Systemes www.3ds.com/products-services/simulia	$$$
Diffpack	inuTech GmbH www.diffpack.com	$$$