

More Examples of the Need for Numerical Methods

Root finding. Figure out how long you need to own a house before it pays to refinance.

Mathematical formulation. Solve the following equation for t

$$c_1(t) - c_2(t) = 0,$$

where $c_1(t)$ is my net cost if I refinance and $c_2(t)$ is my net cost if I don't.

Interpolation. In a CAD system, find the equation of a smooth curve that goes through a set of points indicated by mouse clicks.

Mathematical formulation. Given interpolation points x_1, \dots, x_n ; data values y_1, \dots, y_n ; and basis function $b_1(x), \dots, b_n(x)$. Find coefficients $\alpha_1, \dots, \alpha_n$ such that $\sum_{j=1}^n \alpha_j b_j(x_i) = y_i$, $i = 1, \dots, n$. Or, written as a matrix problem: solve $B\alpha = y$ for α , where $[B]_{ij} = b_j(x_i)$.

Numerical Differentiation. Given the population of tigers in India over the last 10 years, estimate the rate at which that population is decreasing.

Mathematical formulation. Given $(t_i, p(t_i))$ for $i = 1, \dots, n$, estimate $p'(t_n)$.

Numerical ODEs. Simulate the motion of millions of atoms in a crystal.

Mathematical formulation. Give the (x, y, z) coordinate of every atom at time t_0 compute their velocities (and from that, their new positions at time $t_0 + \delta t$) by solving

$$\frac{dv}{dt} = m^{-1} f(x, y, z, t),$$

where $f(x, y, z, t)$ is a really complicated function that depends on the properties of the atoms and on their positions with respect to all the other atoms.

Aproximation. Draw conclusions from some noisy survey data that is supposed to show the influence of major and GPA on expected starting salary of Virginia Tech grads.

Mathematical formulation. The model: $Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2}$, for $i = 1, \dots, m$. Find the "least squares solution" $(\beta_0, \beta_1, \beta_2)$ minimizing

$$\sum_{i=1}^m [Y_i - (\beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2})]^2 = \|r\|_2^2,$$

where

$$r = y - X\beta = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_m \end{bmatrix} - \begin{bmatrix} 1 & X_{11} & X_{12} \\ 1 & X_{21} & X_{22} \\ \vdots & \vdots & \vdots \\ 1 & X_{m1} & X_{m2} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}.$$

Numerical PDEs. Simulate a high strain-rate manufacturing process.

Mathematical formulation.

$$\text{Balance of mass:} \quad (\rho J(1-f))^\cdot = 0, \quad (1)$$

$$\text{Balance of linear momentum:} \quad \rho_r(1-f_r)\dot{\mathbf{v}} = \text{Div } \mathbf{T}, \quad (2)$$

$$\text{Balance of moment of momentum:} \quad \mathbf{T}\mathbf{F}^T = \mathbf{F}\mathbf{T}^T, \quad (3)$$

$$\text{Balance of internal energy:} \quad \rho_r \dot{e} = \rho_r(1-f)[c\dot{\theta} + \text{tr}(\boldsymbol{\sigma}\mathbf{D}^e)] = -\text{Div } \mathbf{Q} + \text{tr}(\mathbf{T}\dot{\mathbf{F}}^T). \quad (4)$$

Where

$$\mathbf{D} = \mathbf{D}^e + \mathbf{D}^\theta + \mathbf{D}^p, \quad (5)$$

$$\mathbf{D}^p = \frac{(1-f)\sigma_m \dot{\varepsilon}_m^p}{\text{tr}(\boldsymbol{\sigma}\mathbf{N}^T)} \mathbf{N}, \quad \mathbf{D} = (\text{grad } \mathbf{v} + (\text{grad } \mathbf{v})^T)/2, \quad \mathbf{D}^\theta = \alpha \dot{\theta} \mathbf{1}, \quad (6)$$

$$\dot{\boldsymbol{\sigma}} + \boldsymbol{\sigma}\boldsymbol{\Omega} - \boldsymbol{\Omega}\boldsymbol{\sigma} = \frac{E(1-f)}{1+\nu} \mathbf{D}^e + \frac{E\nu(1-f)}{(1+\nu)(1-2\nu)} (\text{tr}(\mathbf{D}^e)) \mathbf{1}, \quad (7)$$

$$\mathbf{N} = \frac{3}{\sigma_m^2} \left(\boldsymbol{\sigma} - \frac{1}{3} (\text{tr} \boldsymbol{\sigma}) \mathbf{1} \right) + \frac{f^* q_1 q_2}{\sigma_m} \left[\sinh \left(\frac{q_2 \text{tr} \boldsymbol{\sigma}}{2\sigma_m} \right) \right] \mathbf{1}, \quad (8)$$

$$\Phi \equiv \frac{3}{2} \frac{\text{tr}(\mathbf{s}\mathbf{s}^T)}{\sigma_m^2} + 2f^* q_1 \cosh \left(\frac{q_2 \text{tr} \boldsymbol{\sigma}}{2\sigma_m} \right) - 1 - q_1^2 f^{*2} = 0, \quad \mathbf{s} = \boldsymbol{\sigma} - \frac{1}{3} (\text{tr} \boldsymbol{\sigma}) \mathbf{1}, \quad (9)$$

$$f^* = \begin{cases} f & \text{if } f \leq f_c, \\ f_c + \left(\frac{f_u^* - f_c}{f_f - f_c} \right) (f - f_c), & f > f_c, \end{cases} \quad (10)$$

$$\dot{\varepsilon}_m^p = \max \left[0, \frac{1}{b} \left\{ \left(\frac{\sigma_m}{\sigma_0 \left(1 + \frac{\varepsilon_m^p}{\varepsilon_0} \right)^n (1 - \beta\theta)} \right)^{\frac{1}{m}} - 1 \right\} \right], \quad (11)$$