The Hidden Role of Mathematics and Computation in Scientific Discovery and Engineering

Summer Sessions
Groundbreaking Research / Innovative Technology
GRIT Series

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Impact of Mathematics (a few examples):

- **Internet Services**: Search, Streaming, Encryption, Machine Learning.
- **Cell Phones**: Design, Materials, Data Compression.
- **Scientific Investigations**: Modeling, Simulation, Data Analysis.
Cell Phone Cameras and Pictures

- Typical cell phone camera: 16 megapixels (millions of pixels).
- Direct storage/transmission of information not practical (raw image ~ 48MB, 24-bit color).
- Means 1 GB ~ only 20 images could be stored or transmitted!

Compression

- Only subset of features of the image are perceived when viewing.
- Need good mathematical ways to process and discard less perceptible features.
- If we can achieve even 10:1 compression then 1GB ~ 200 images stored or transmitted!
- Image compression methods ← JPEG currently most widely used standard.
Part I : Image Compression
Visual Perception: Models to Represent Color

Human Vision and Color Perception

Response of S, M, L Cones

CIE 1931 Color Space Model
(colors visible to human eye)

Colors that can be generated
by typical RGB display

Image

Pixels

RGB Color Cube

Y’C’B’C’ Color Space

Pixel RGB Values

R = 0.59
G = 0.54
B = 0.71

\[ Y' = K_R \cdot R' + (1 - K_R - K_B) \cdot G' + K_B \cdot B' \]

\[ C_B = \frac{C}{2} \cdot \frac{B' - Y'}{1 - K_B} \]

\[ C_R = \frac{C}{2} \cdot \frac{R' - Y'}{1 - K_R} \]
Color Representations: RGB → Y'CbCr

Linear Transform: RGB → Y'CbCr

\[
Y' = K_R \cdot R' + (1 - K_R - K_B) \cdot G' + K_B \cdot B'
\]

\[
C_B = \frac{C \cdot B' - Y'}{2 \cdot (1 - K_B)}
\]

\[
C_R = \frac{C \cdot R' - Y'}{2 \cdot (1 - K_R)}
\]

Y'CbCr Color Space

Quantization
Perception: Primarily Smooth Variations

Discrete Cosine Transform (DCT) [2D]
JPEG Images and Discrete Fourier Transforms

**Discrete Cosine Transform (DCT)**

\[ X_k = DCT[x_n] = \sqrt{\frac{2}{N}} \sum_{n=0}^{N-1} x_n \cos \left( \frac{\pi}{N} \left( n + \frac{1}{2} \right) k \right) \]

\[ k = 0, \ldots, N - 1 \]

**Inverse Discrete Cosine Transform (iDCT)**

\[ x_n = iDCT[x_n] = \sqrt{\frac{2}{N}} \left( \frac{X_0}{2} + \sum_{k=1}^{N-1} X_k \cos \left( \frac{\pi}{N} \left( n + \frac{1}{2} \right) k \right) \right) \]

**Pixel Intensity 2D**

\[ x_{m,n} = iDCT_{\ell}^k [iDCT_{\ell}^k [X_{k\ell}]] \]

\[ x_{m,n} = DCT_{\ell}^k [DCT_{\ell}^k [x_{mn}]] \]
JPEG Protocol

- RGB image data transformed to YCₐCₐ color space and quantize (drop bits).
- Transform by DCT 8x8 blocks to frequency space.
- Frequency coefficients are quantized (stored with less bits) [Q controlled].
- Remaining data is entropy encoded (lossless compression).
- Final result is JPEG file. What is compression achieved in practice?
JPEG Images

Compression Ratio = 6:1
Quality = 50%

Compression Ratio = 18:1
Quality = 10%

Compression Ratio = 51:1
Quality = 1%
Impact of Mathematics (a few examples):

- **Internet Services:** Search, Streaming, Encryption, Machine Learning.
- **Cell Phones:** Design, Materials, Data Compression.
- **Engineering:** Design, Virtual Testing, Optimization, Elasticity, Fluid-Structure Interaction.
- **Scientific Investigations:** Modeling, Simulation, Data Analysis.
Part II: Stochastic Modeling and Scientific Computation
Central Limit Theorem

\[ \mu < \infty \quad \sigma^2 < \infty \]

\[ \frac{\sum_{k=1}^{N} (X_k - \mu)}{\sigma \sqrt{N}} \rightarrow \eta(0, 1) \]

Gaussian Distribution

\[ \rho(x) = \frac{1}{\sqrt{2\pi}} \exp \left( -\frac{x^2}{2} \right) \]

Normal Distribution: Gauss’ Curve

Coin Flips

Dice Rolls

Other Phenomena:

Height of Ocean Waves

SAT Exam Scores

N. Borge 2014

P. Hoffmann 2014

D. Ma 2011

Mean

\[ \mu = E[X] = \sum_i x_i p_i \]

Variance

\[ \sigma^2 = E[(X - \mu)^2] = \sum_i (x_i - \mu)^2 p_i \]
Brownian Motion

Contributions:

• 1827: R. Brown: observes erratic motions of pollen grains of plant *Clarkia pulchella*.

• 1905: Einstein: theory of Brownian motion: links diffusivity D to mechanical drag, temperature.

• 1908/1915: Langevin / Smoluchowski develop theories in classical mechanics with random forces.

• ~1930’s: Wiener develops mathematical foundations (measure theory on function spaces / non-diff).
Brownian Motion

Langevin Equation \((\text{ma} = \text{F})\)

\[
m \frac{dV}{dt} = -\gamma V + -\nabla \Phi + F_{\text{thm}}
\]

\(F_{\text{thm}}(s) \sim \text{Gaussian}\)

\[
\langle F_{\text{thm}}(s) F_{\text{thm}}(t) \rangle = 2k_B T \gamma \delta(t - s)
\]

Hydrodynamics + Fluctuations

Colloids / Suspensions

Polymers

Membranes (lipids)

Cell Biology
**Stochastic Immersed Boundary Method**

**Fluid-structure equations**

Fluid:
\[
\rho \frac{D\mathbf{u}(x, t)}{Dt} = \mu \Delta \mathbf{u}(x, t) - \nabla p(x, t) + \mathbf{F}_{\text{prt}}(x, t)
\]
\[
\nabla \cdot \mathbf{u}(x, t) = 0.
\]

Microstructure:
\[
\frac{dX^{[j]}(t)}{dt} = \int \delta_a(x - X^{[j]}(t))\mathbf{u}(x, t)dx
\]
\[
\mathbf{F}_{\text{prt}}(x, t) = \sum_{j=1}^{M} \mathbf{F}^{[j]} \delta_a \left( x - X^{[j]}(t) \right)
\]

**Numerical Discretization**

**Fluid-Structure Coupling**

**Thermal fluctuations**

\[
\mathbf{F}_{\text{thm}}(x, t) = \mathbf{F}_{\text{drift}}(x, t) + \mathbf{F}_{\text{stoch}}(x, t) \sim \text{Gaussian}
\]
\[
\langle \mathbf{F}_{\text{stoch}}(x, t)\mathbf{F}_{\text{stoch}}^T(y, s) \rangle = -2k_B T \mu \Delta \delta(x - y)\delta(t - s)
\]
\[
\mathbf{F}_{\text{drift}} = -k_B T \sum_{j=1}^{M} \nabla X^{[j]} \delta_a(x - X^{[j]}(t))
\]

Rheological Properties and Microstructure Dynamics

Rheometry:

Polymeric Fluid (FENE)

$$U(r) = \frac{K}{2} Q_0^2 \log \left(1 - \frac{r}{Q_0}\right)^2$$

Shear Viscosity

$$\eta_p = \frac{\sigma_{(a,a)}}{\dot{\gamma}}$$

Lees-Edwards Conditions:

Material Stress $\leftrightarrow$ Forces

Polymeric Material

Forces

$$\sigma_{\xi,z}^{(n)} = \frac{1}{AL} \sum_{q \in Q_n} \sum_{j=1}^{n-1} \left[ \langle \epsilon^{(q)}_{\xi,j} \rangle \left( x_{q_n}^{(q)}(z) - x_{q_j}^{(q)}(z) \right) \right]$$
Lipid Bilayer Membranes: Coarse-Grained Modeling

Cell Biology / Biophysics

Lipid Interactions

Coarse-Grained Model

Lipid Bilayer Membranes

SIB/SELM Model

Correlation Analysis

Two-point correlation

Results

Langevin: Stokes Drag

SELM: Fluctuating Hydrodynamics
Conclusions

Internet Services

Cell Phone

Engineering

Scientific Investigations

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**Mathematics broad impact.**

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**Future Studies / Career**

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**Best Jobs: (Wall Street Journal 2011)**

1. Mathematician
2. Actuary
3. Statistician
4. Biologist
5. Software Engineer
6. Computer Systems Analyst

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**Math Increasingly Central**