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

Summer Sessions

Groundbreaking Research / Innovative Technology
GRIT Series

July 2016

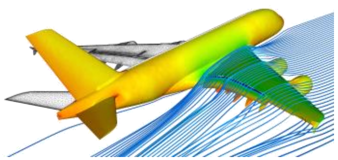
Paul J. Atzberger
Department of Mathematics
Department of Mechanical Engineering
University of California Santa Barbara

Mathematics in Modern Technology and Science

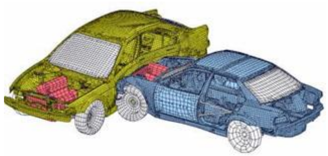
Internet Services

Cell Phone

Engineering

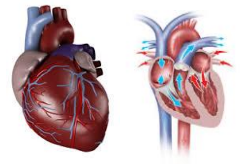


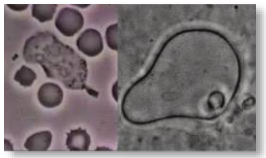
Texas A&M : Transportation Institute (TTI)



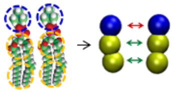
Computer Simulation : ICT

Scientific Investigations

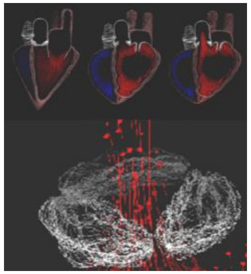




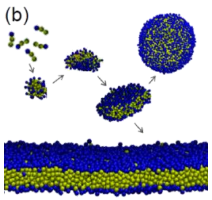
David Rogers



Deserno et al.



Peskin,C and McQueen, D. et al.
Griffith et al.



Atzberger, P.,Sigurdsson, J. et al.

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.

Cell Phones, Images, and Data Compression

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!

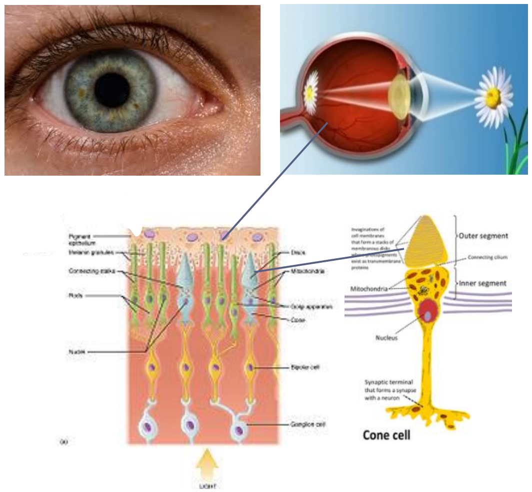
Compression

- 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.

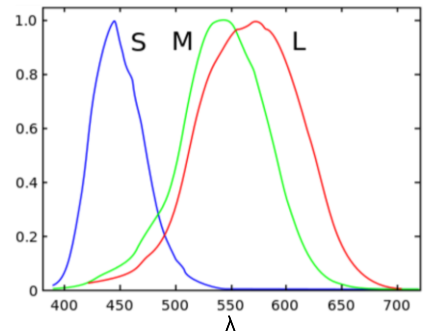
Part I : Image Compression

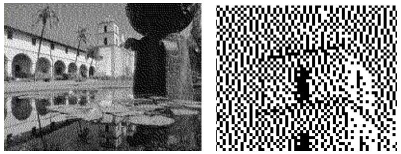
Visual Perception : Models to Represent Color

Human Vision and Color Perception

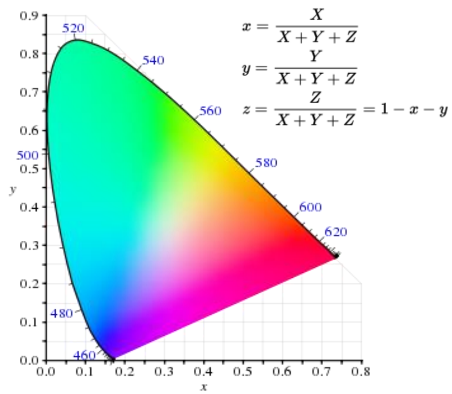


Response of S,M,L Cones

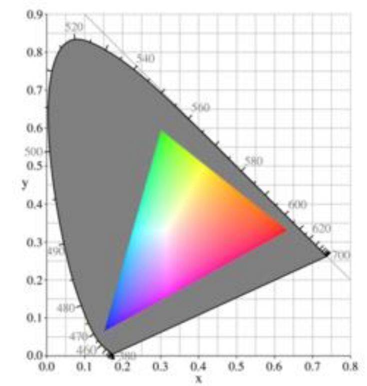




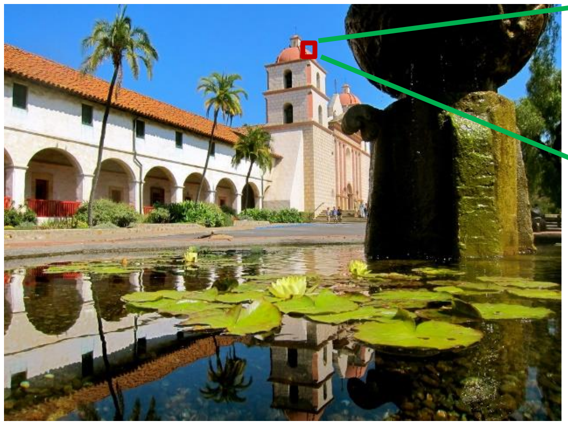
CIE 1931 Color Space Model (colors visible to human eye)



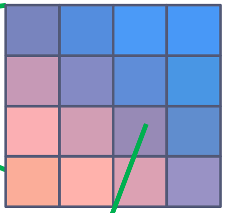
Colors that can be generated by typical RGB display

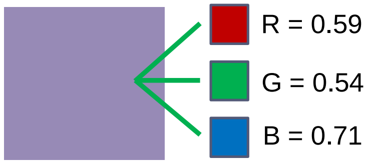


Image



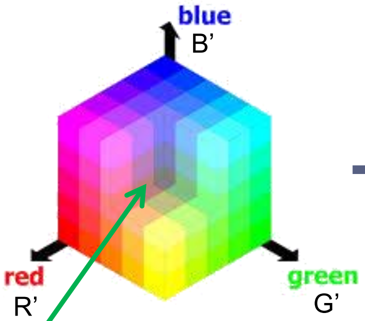
Pixels



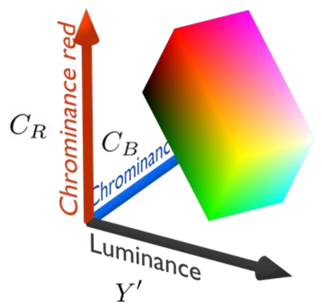


Pixel RGB Values

RGB Color Cube



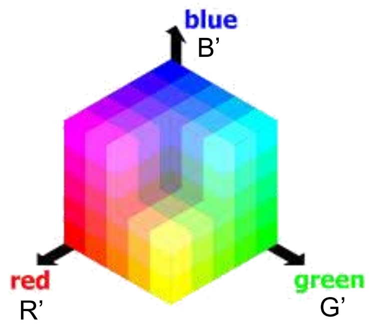
Y'$C_B$$C_R$ Color Space



$$Y' = K_R \cdot R' + (1 - K_R - K_B) \cdot G' + K_B \cdot B'$$
$$C_B = \frac{C}{2} \cdot \frac{B' - Y'}{1 - K_B}$$
$$C_R = \frac{C}{2} \cdot \frac{R' - Y'}{1 - K_R}$$

Color Representations : RGB → Y'$C_B C_R$

RGB Color Cube

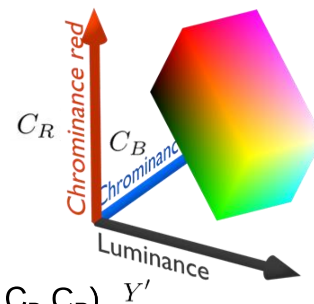


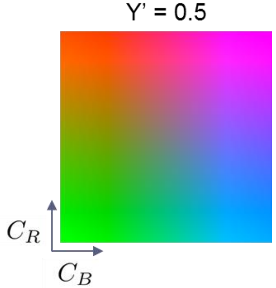
Linear Transform: RGB → Y'$C_B C_R$

$$Y' = K_R \cdot R' + (1 - K_R - K_B) \cdot G' + K_B \cdot B'$$
$$C_B = \frac{C}{2} \cdot \frac{B' - Y'}{1 - K_B}$$
$$C_R = \frac{C}{2} \cdot \frac{R' - Y'}{1 - K_R}$$

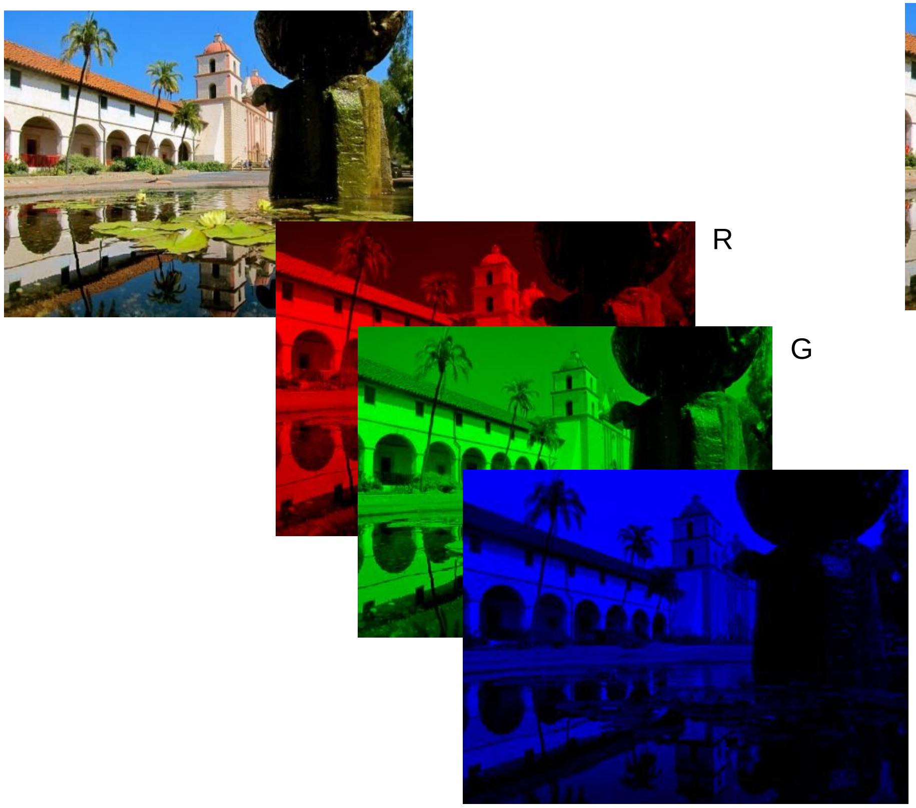
(R',G',B') → (Y',C_B,C_R)

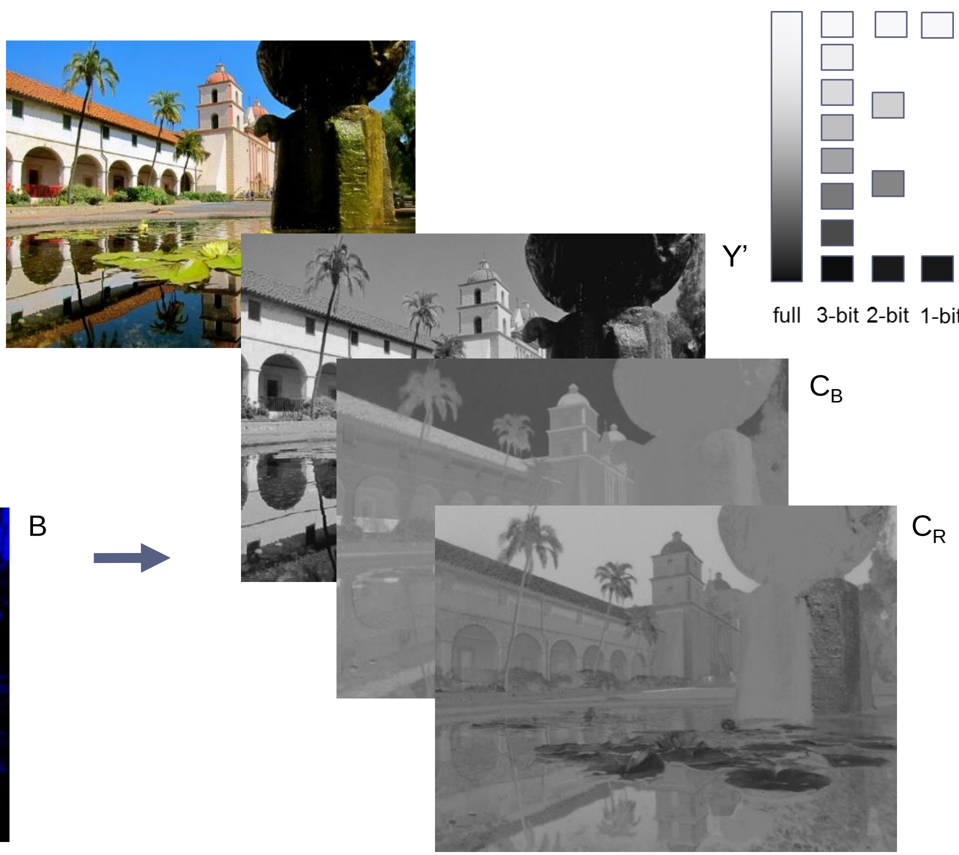
Y'$C_B C_R$ Color Space



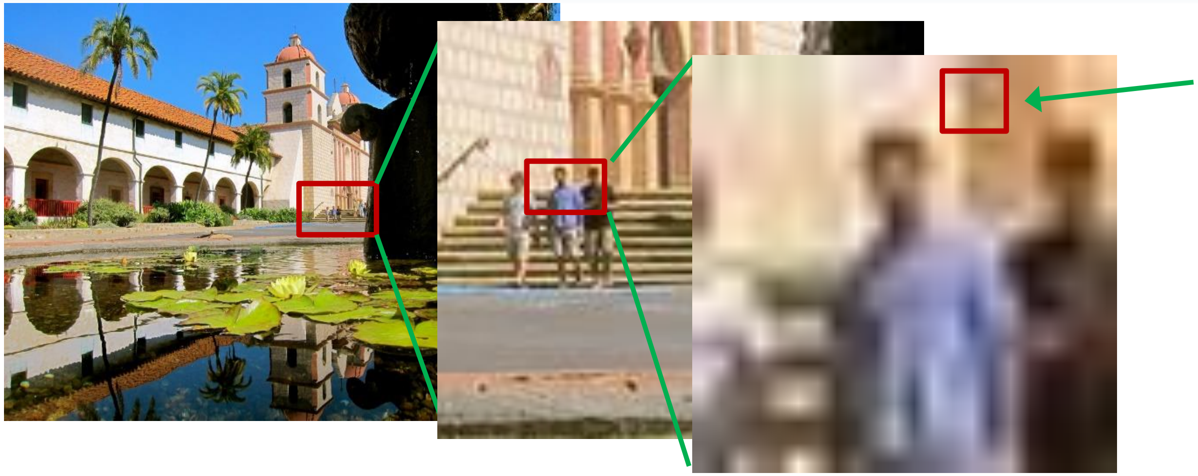


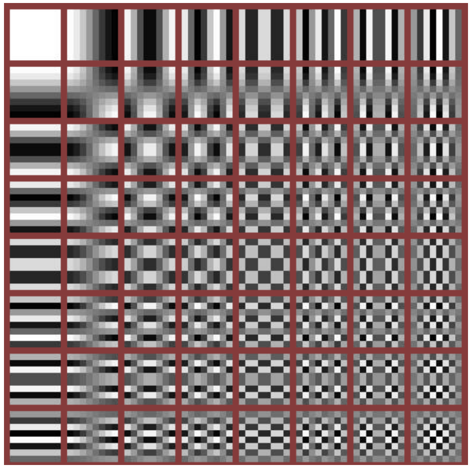
Quantization



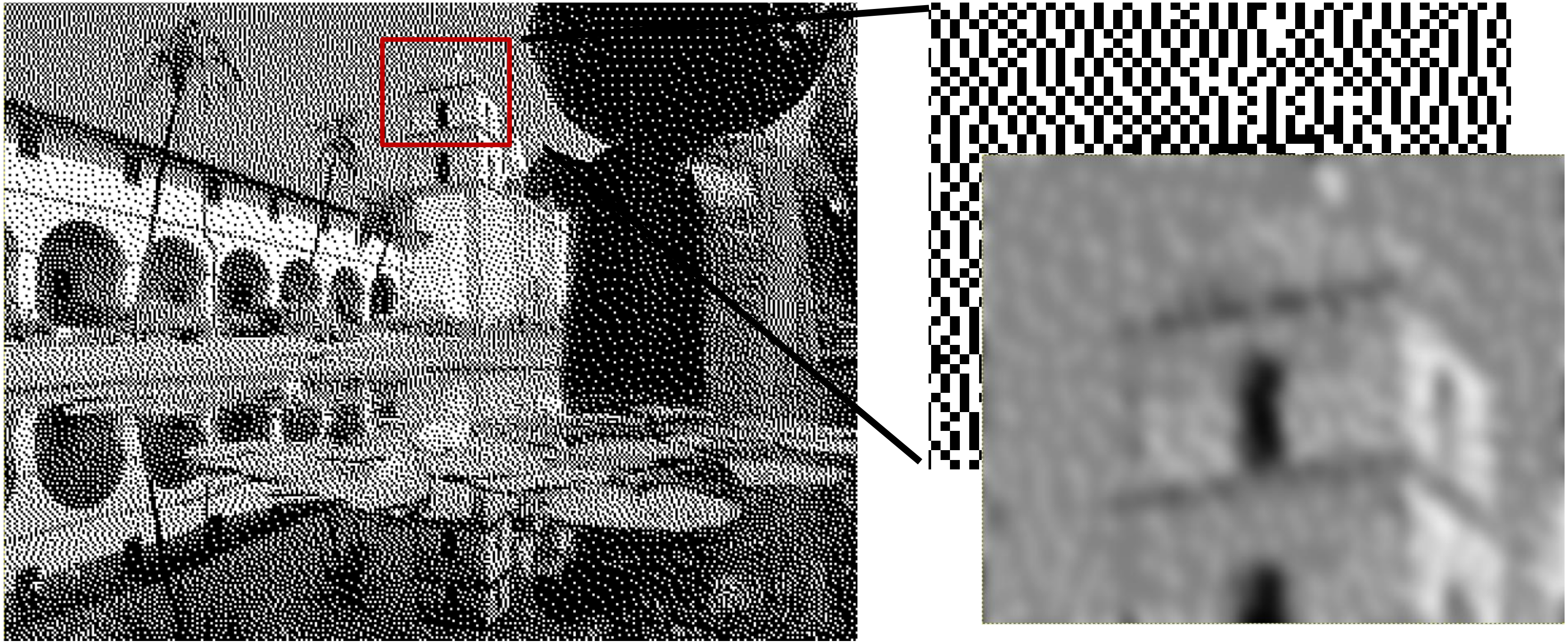


Perception : Primarily Smooth Variations

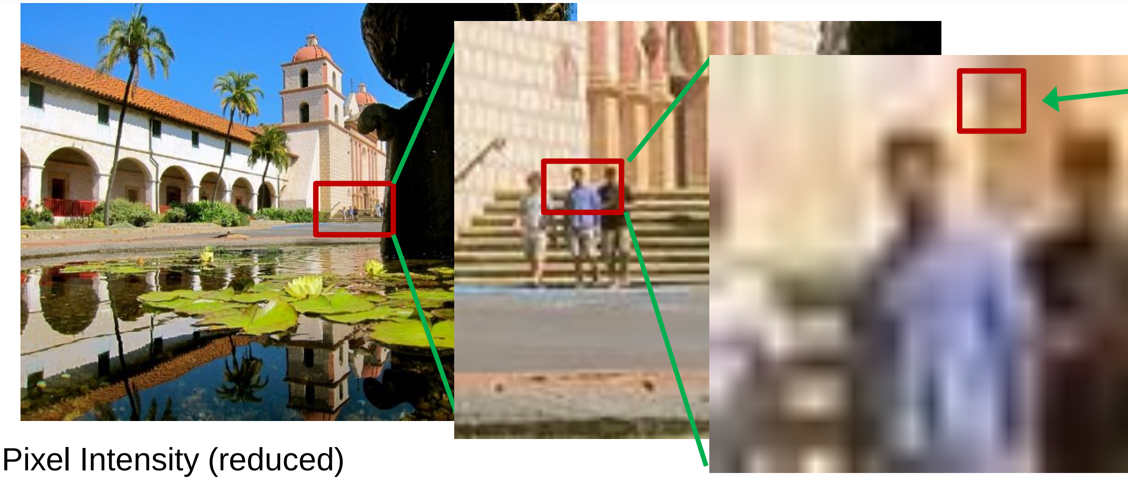


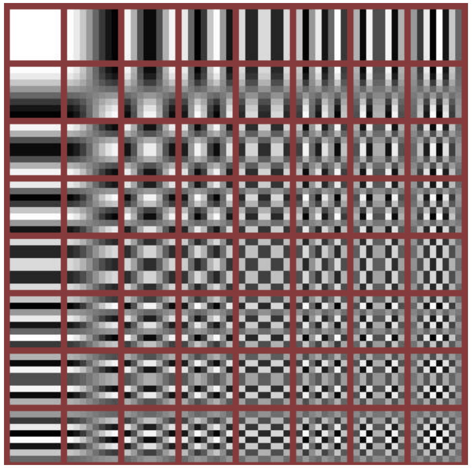


Discrete Cosine Transform (DCT) [2D]



JPEG Images and Discrete Fourier Transforms



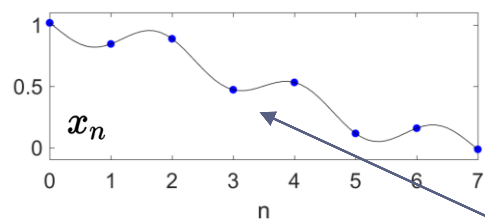


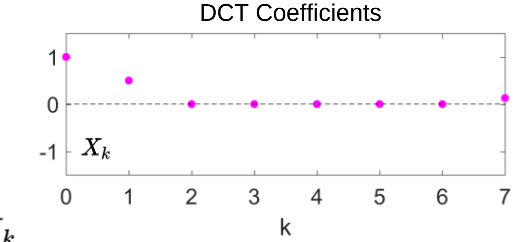
Discrete Cosine Transform (DCT) [2D]

Pixel Intensity (reduced)

Pixel Intensity

0 x_n 7





X_k

Discrete Cosine Transform (DCT)

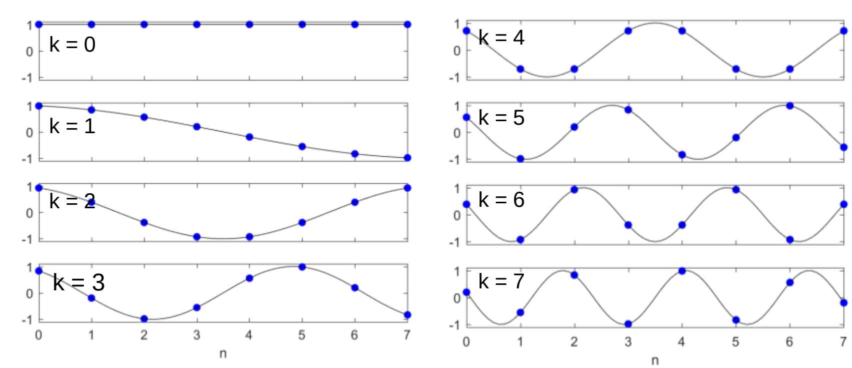
$$X_k = DCT[x_n] = \sqrt{\frac{2}{N}} \sum_{n=0}^{N-1} x_n \cos\left[\frac{\pi}{N}\left(n+\frac{1}{2}\right)k\right]$$

$$k = 0, \dots, N-1$$

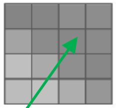
Inverse Discrete Cosine Transform (iDCT)

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

DCT Modes



Pixel Intensity 2D **Discrete Cosine Transform (DCT) [2D]**

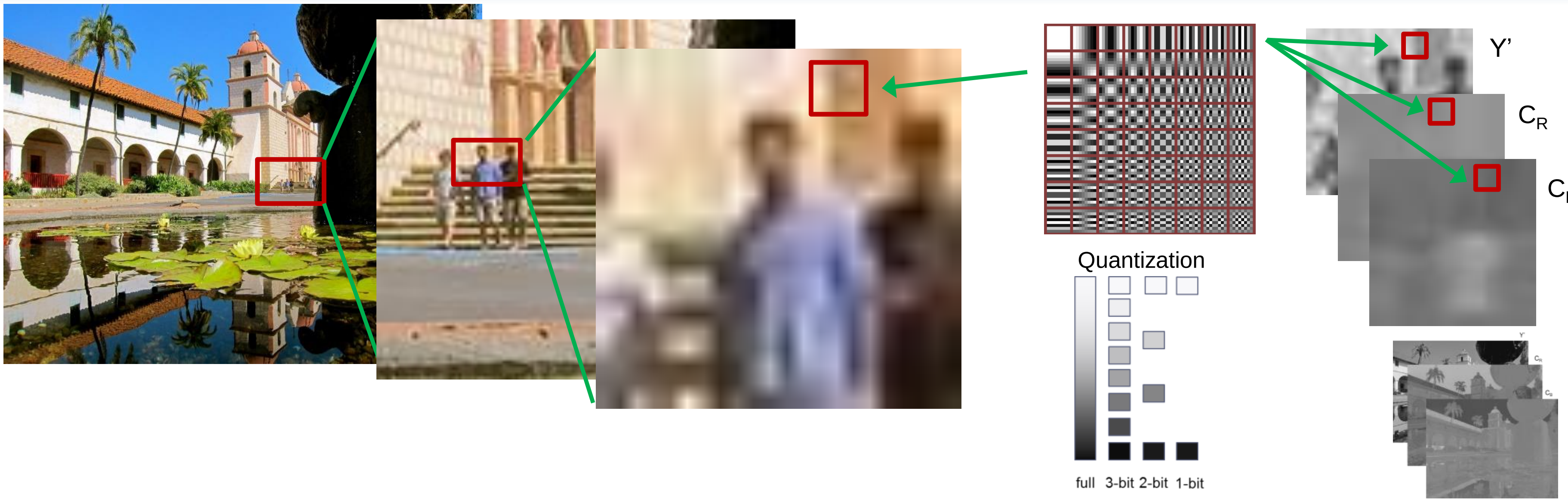


$x_{m,n}$

$$X_{k\ell} = DCT_m^{\ell}[DCT_n^{k}[x_{mn}]]$$

$$x_{mn} = iDCT_k^{\ell}[iDCT_{\ell}^{k}[X_{k\ell}]]$$

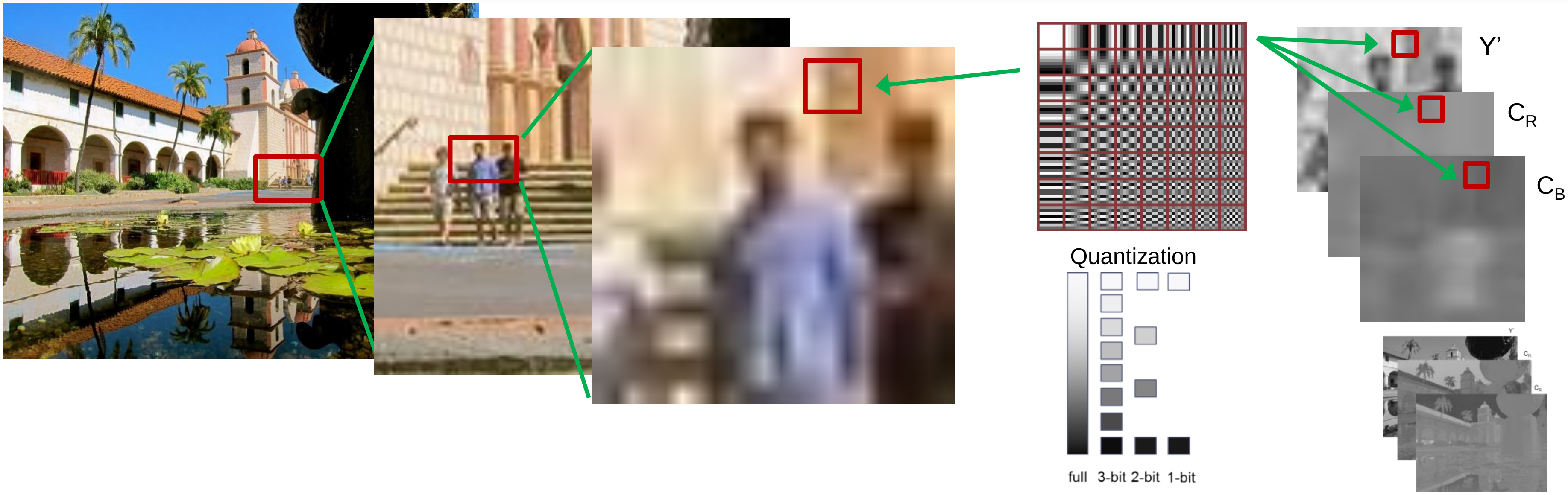
JPEG Compression Protocol



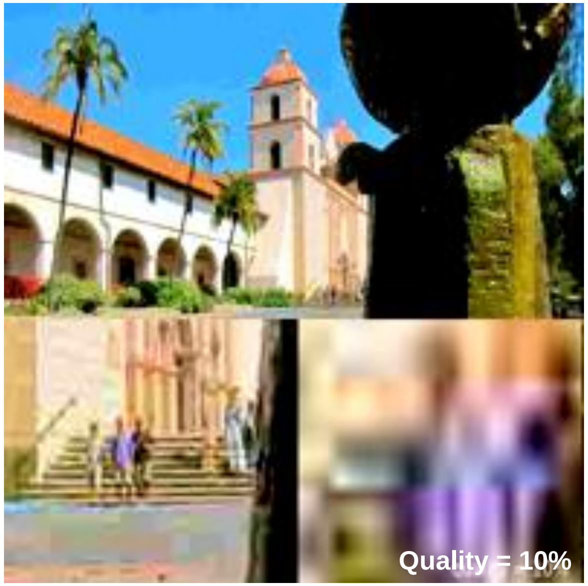
JPEG Protocol

- RGB image data transformed to YC_BC_R 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



Compression Ratio = 18:1

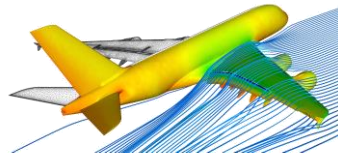
Compression Ratio = 51:1

Mathematics in Modern Technology and Science

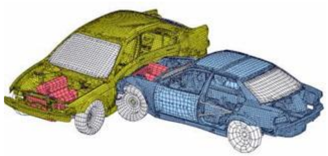
Internet Services

Cell Phone

Engineering

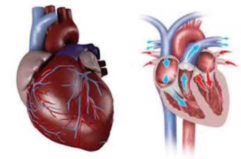


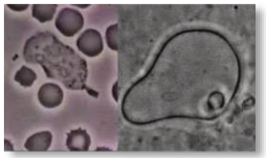
Texas A&M : Transportation Institute (TTI)



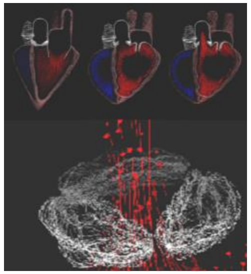
Computer Simulation : ICT

Scientific Investigations

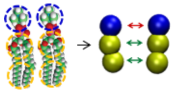




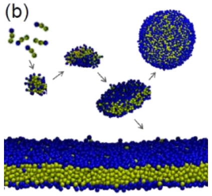
David Rogers



Peskin,C and McQueen, D. et al.
Griffith et al.



Deserno et al.



Atzberger, P.,Sigurdsson, J. et al.

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.

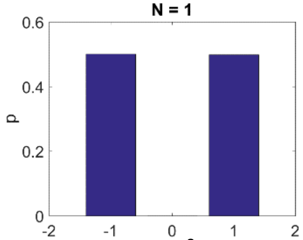
Part II : Stochastic Modeling and Scientific Computation

Normal Distribution: Gauss' Curve

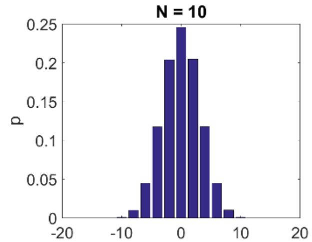
Coin Flips

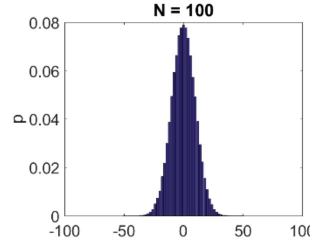
+1

-1



$\mu=0,\ \sigma^2=1$





Mean

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

Variance

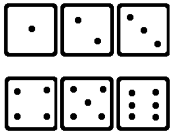
$$\sigma^2 = E[(X-\mu)^2] = \sum_i (x_i - \mu)^2 p_i$$

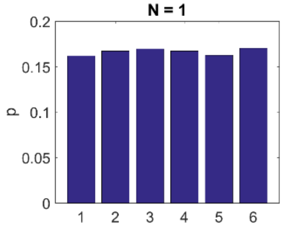
Central Limit Theorem

$$\mu < \infty \qquad \sigma^2 < \infty$$

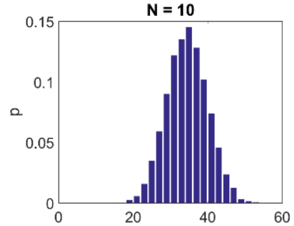
$$\frac{\sum_{k=1}^{N}(X_k - \mu)}{\sigma\sqrt{N}} \to \eta(0,1)$$

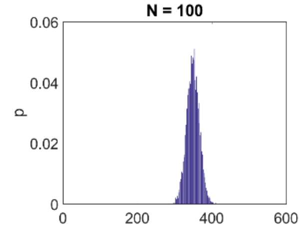
Dice Rolls

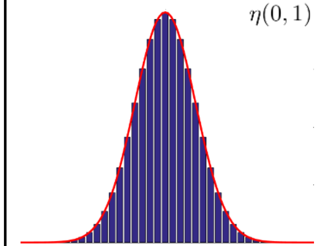




$\mu=3.5,\ \sigma^2=2.9$





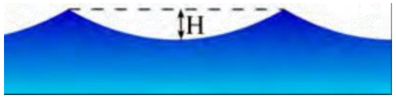


Gaussian Distribution

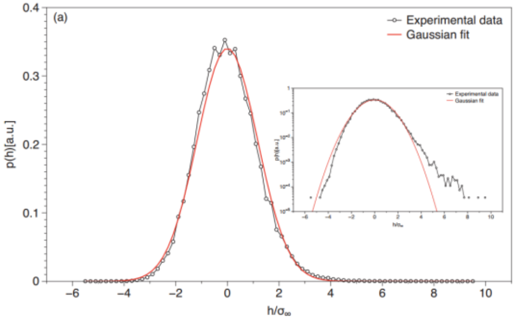
$$\rho(x) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{x^2}{2}\right]$$

Other Phenomena:

Height of Ocean Waves

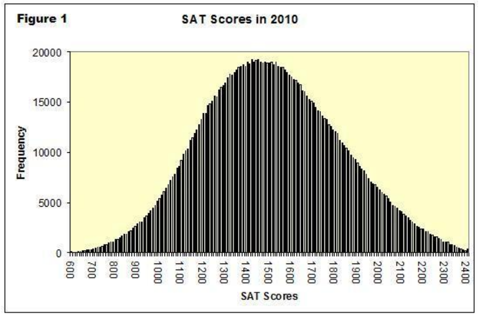


N. Borge 2014



P. Hoffmann 2014

SAT Exam Scores

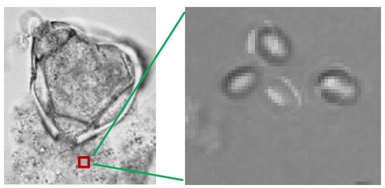


D. Ma 2011

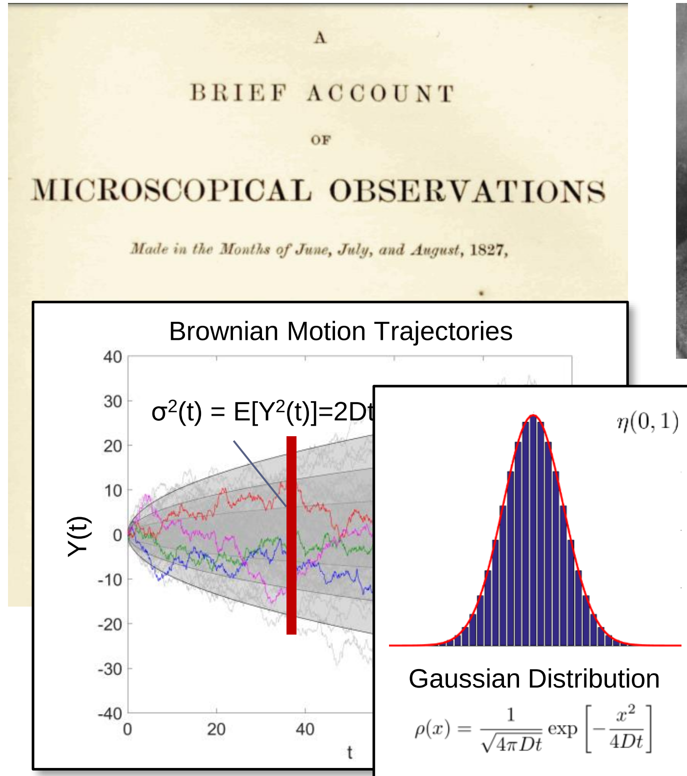
Brownian Motion

Robert Brown
1773 –1858

Clarkia pulchella



Pearle 2010



A

BRIEF ACCOUNT

OF

MICROSCOPICAL OBSERVATIONS

Made in the Months of June, July, and August, 1827,

Alber

Pau

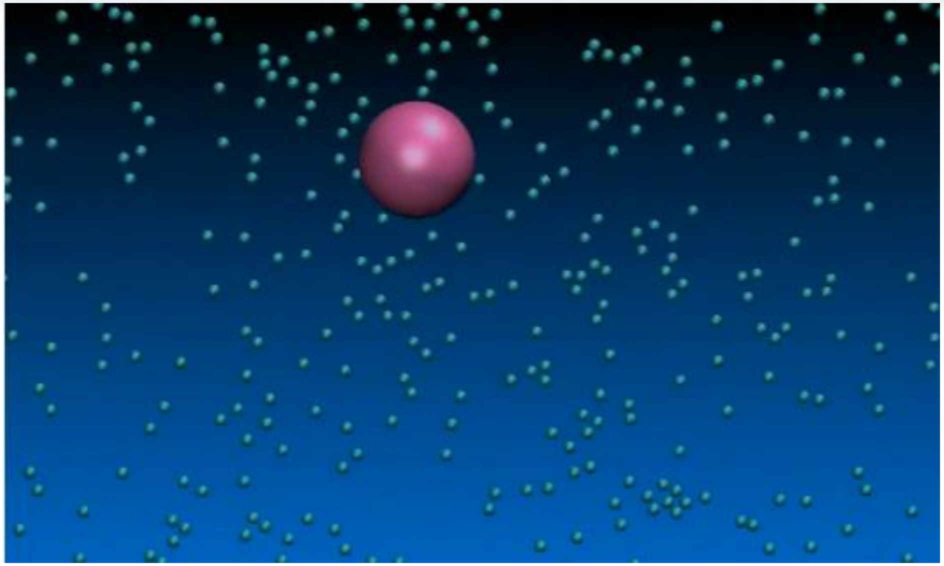
Maria

Norbert Wiener

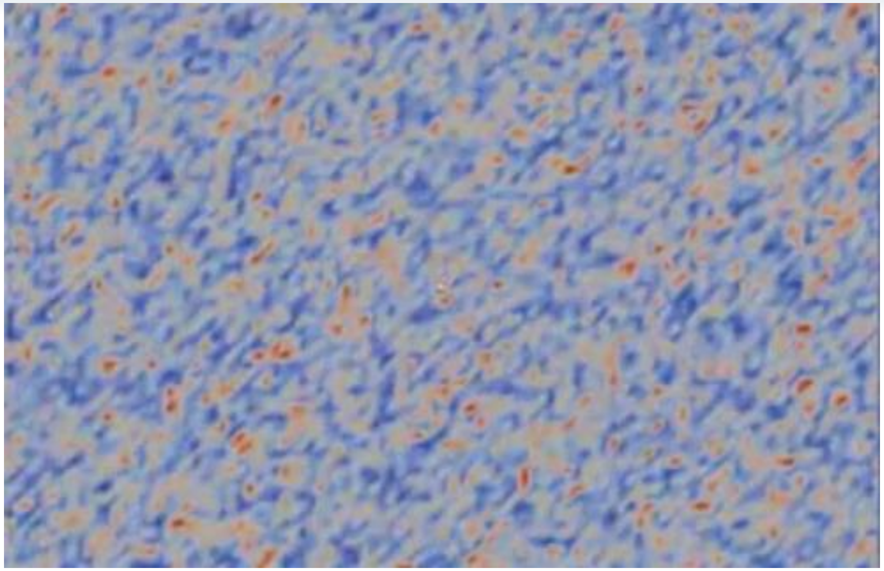
Contributions:

- 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



Brownian Motion: Molecular Collisions



Continuum Gaussian Random Field

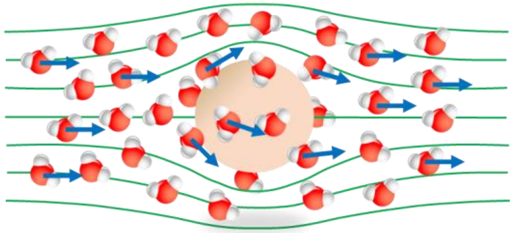
Langevin Equation (ma = F)

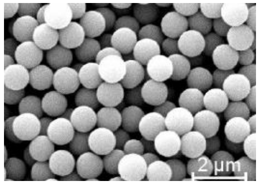
$$m\frac{dV}{dt} = -\gamma V + -\nabla\Phi + F_{\text{thm}}$$

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

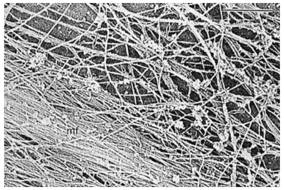
$$\langle F_{\text{thm}}(s)F_{\text{thm}}(t)\rangle = 2k_B T\gamma\delta(t-s)$$

Hydrodynamics + Fluctuations

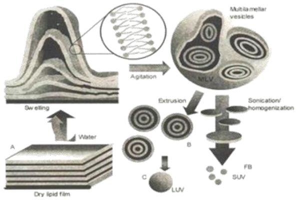




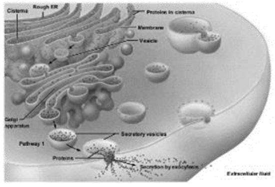
Colloids / Suspensions



Polymers

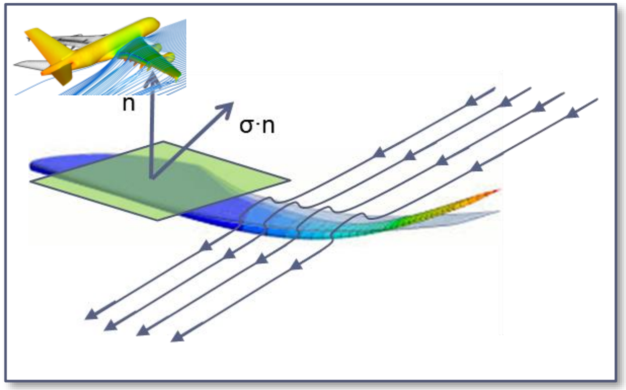


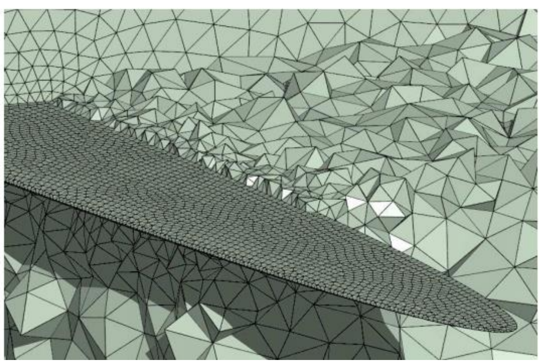
Membranes (lipids)



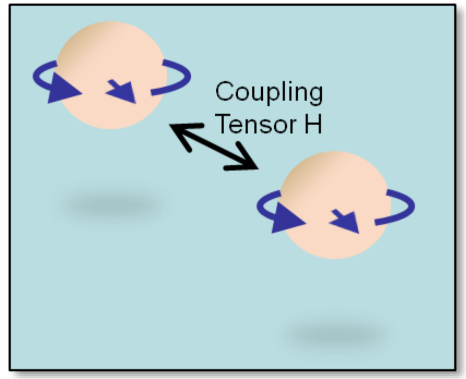
Cell Biology

CFD : Approaches to Fiuid-Structure Interactions

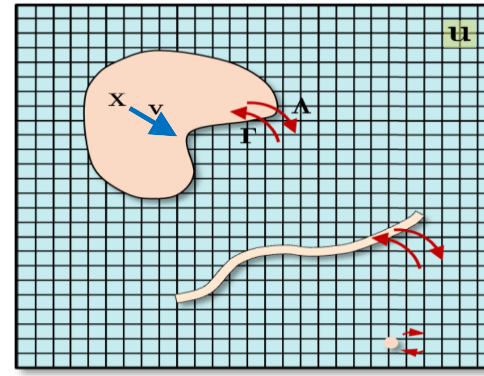


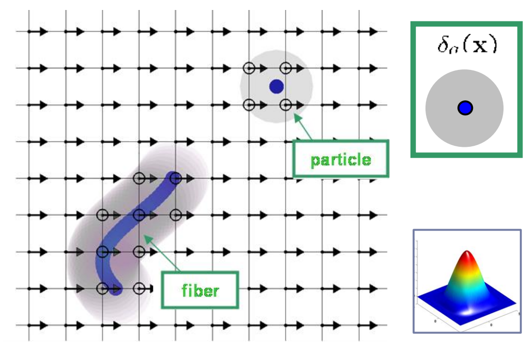


J. Peraire and P.-O. Persson



Brady et al., G. Gompper et al.





Atzberger, Peskin, Kramer

Stochastic Immersed Boundary Method

Fluid-structure equations

Fluid:

$$\rho \frac{D\mathbf{u}(\mathbf{x},t)}{Dt} = \mu \Delta \mathbf{u}(\mathbf{x},t) - \nabla p(\mathbf{x},t) + \mathbf{F}_{\mathrm{prt}}(\mathbf{x},t)$$

$$\nabla \cdot \mathbf{u}(\mathbf{x},t) = 0.$$

Microstructure:

$$\frac{d\mathbf{X}^{[j]}(t)}{dt} = \int \delta_a(\mathbf{x} - \mathbf{X}^{[j]}(t))\mathbf{u}(\mathbf{x},t)d\mathbf{x}$$

$$\mathbf{F}_{\mathrm{ptr}}(\mathbf{x},t) = \sum_{j=1}^{M} \mathbf{F}^{[j]} \delta_a\left(\mathbf{x} - \mathbf{X}^{[j]}(t)\right)$$

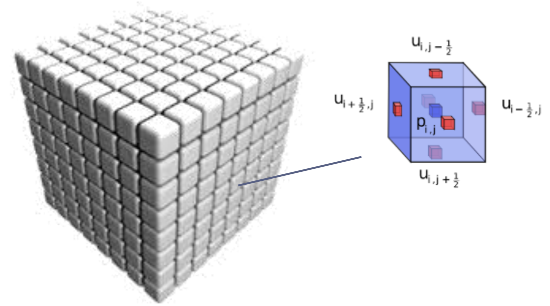
Thermal fluctuations

$$\mathbf{F}_{\mathrm{thm}}(\mathbf{x},t) = \mathbf{F}_{\mathrm{drift}}(\mathbf{x},t) + \mathbf{F}_{\mathrm{stoch}}(\mathbf{x},t) \sim \mathrm{Gaussian}$$

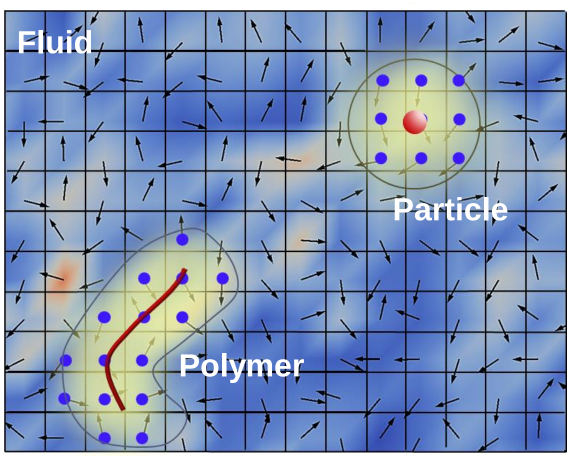
$$\left\langle \mathbf{F}_{\mathrm{stoch}}(\mathbf{x},t)\mathbf{F}_{\mathrm{stoch}}^{T}(\mathbf{y},s)\right\rangle = -2k_B T \mu \Delta \delta(\mathbf{x}-\mathbf{y})\delta(t-s)$$

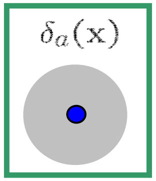
$$\mathbf{F}_{\mathrm{drift}} = -k_B T \sum_{j=1}^{M} \nabla_{\mathbf{X}^{[j]}} \delta_a(\mathbf{x} - \mathbf{X}^{[j]}(t))$$

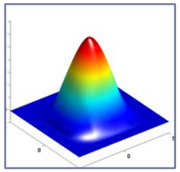
Numerical Discretization



Fluid-Structure Coupling



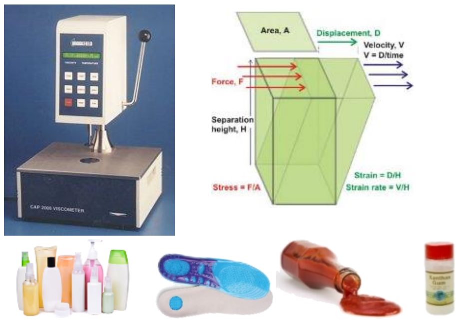




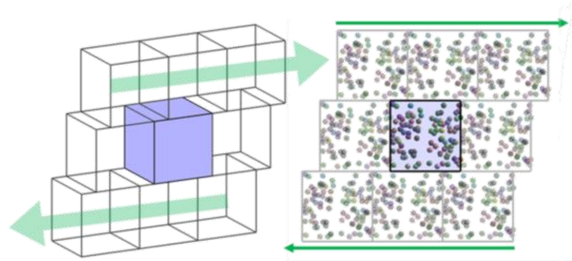
Peskin 1972, Atzberger, Peskin, Kramer 2007, Atzberger, Tabak 2015

Rheological Properties and Microstructure Dynamics

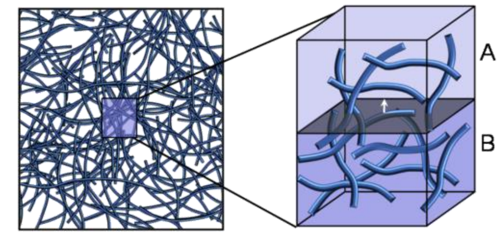
Rheometry:



Lees-Edwards Conditions:



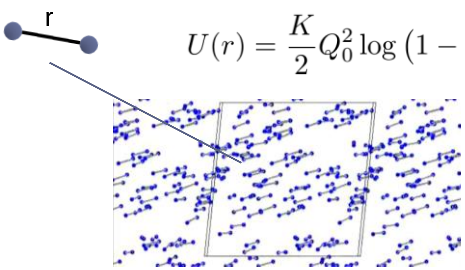
Material Stress ← Forces



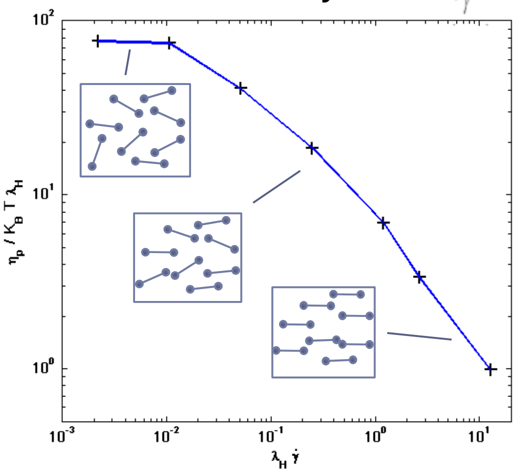
$$\sigma_{\ell,z}^{(n)} = \frac{1}{AL}\sum_{\mathbf{q}\in\mathcal{Q}_n}\sum_{j=1}^{n-1}\left\langle \mathbf{f}_{\mathbf{q},j}^{(\ell)} \cdot \left(\mathbf{x}_{q_n}^{*,(z)} - \mathbf{x}_{q_j}^{*,(z)}\right)\right\rangle$$

Polymeric Fluid (FENE)

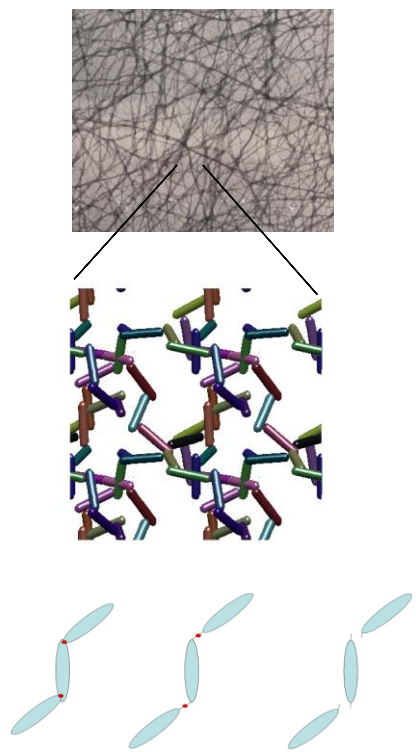
$$U(r) = \frac{K}{2}Q_0^2 \log\left(1 - (r/Q_0)^2\right)$$

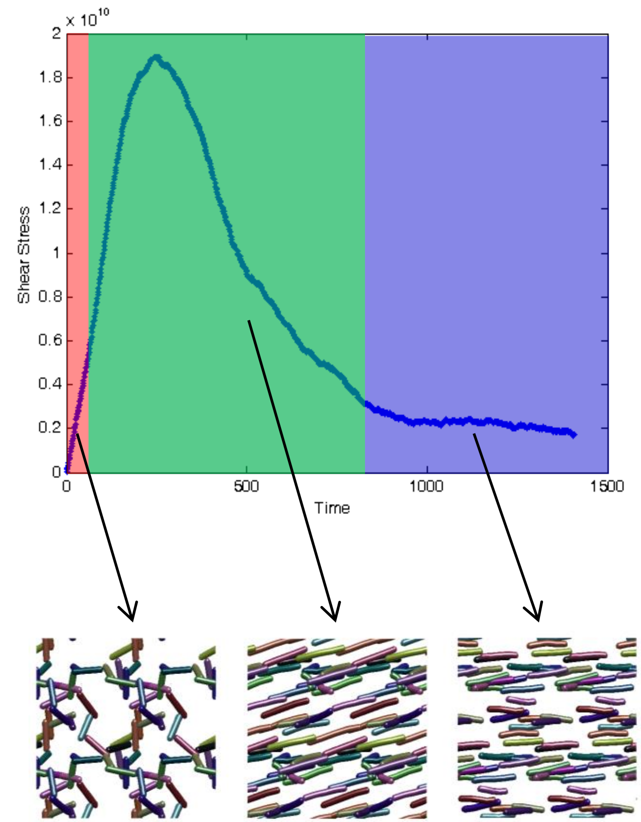


Shear Viscosity $\eta_p = \frac{\sigma^{(s,v)}}{\dot{\gamma}}$



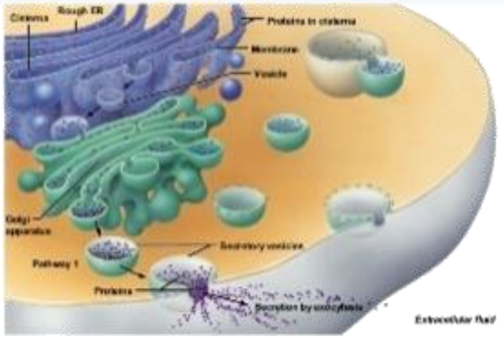
Polymeric Material

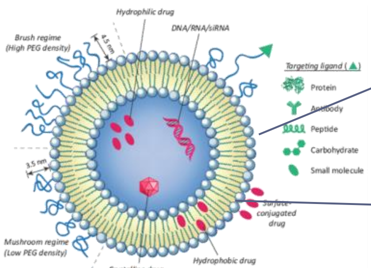


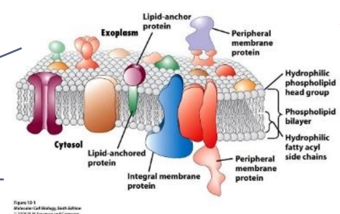


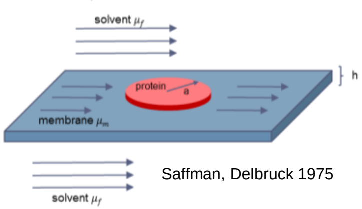
Lipid Bilayer Membranes : Coarse-Grained Modeling

Cell Biology / Biophysics



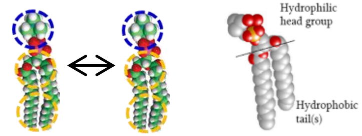




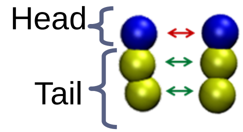


Saffman, Delbruck 1975

Lipid Interactions

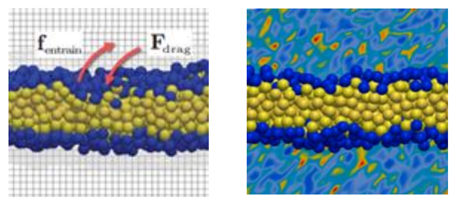


Coarse-Grained Model



Deserno 2005.

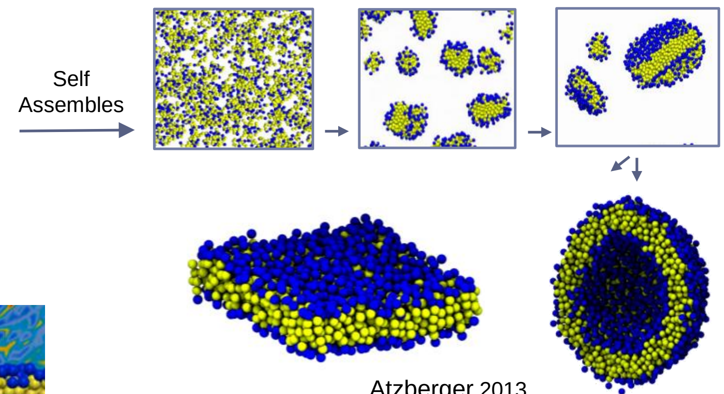
SIB/SELM Model



Lipid Bilayer Membranes

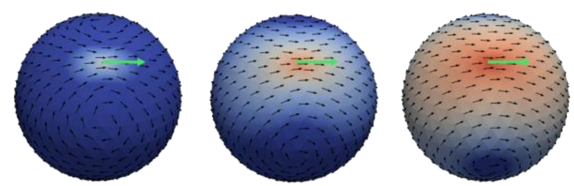
Self-Assembled Bilayers

Self Assembles



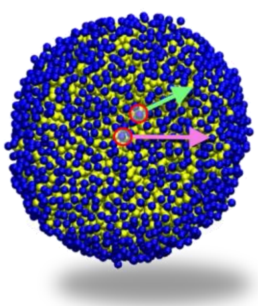
Atzberger 2013.

Atzberger 2016.

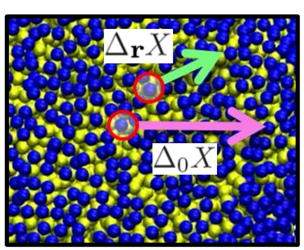


Correlation Analysis

Two-point correlation



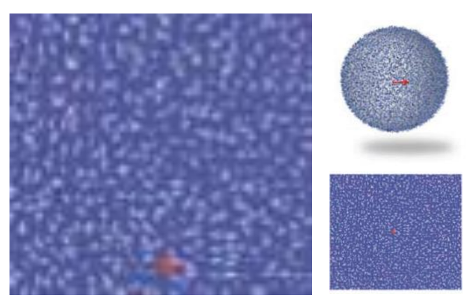
Displacement Δt



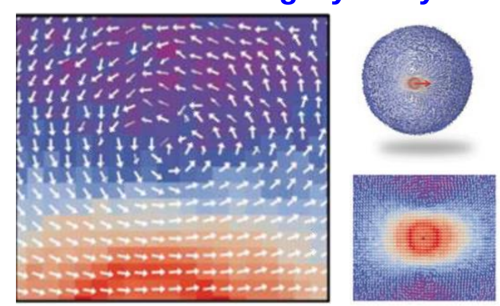
$$\Psi(\mathbf{r}) = \langle \Delta_{\mathbf{r}} X \Delta_0 X^T \rangle$$

Results

Langevin:Stokes Drag



SELM: Fluctuating Hydrodynamics

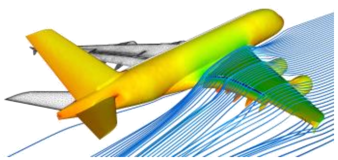


Conclusions

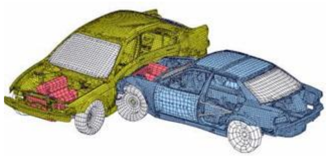
Internet Services

Cell Phone

Engineering

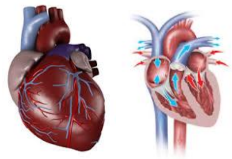


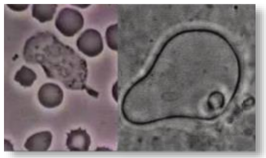
Texas A&M : Transportation Institute (TTI)



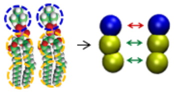
Computer Simulation : ICT

Scientific Investigations

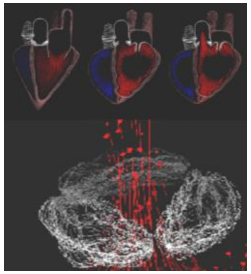




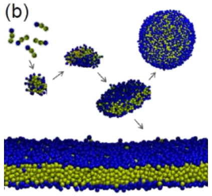
David Rogers



Deserno et al.



Peskin,C and McQueen, D. et al.
Griffith et al.



Atzberger, P.,Sigurdsson, J. et al.

Mathematics broad impact.

Future Studies / Career

Best Jobs: (Wall Street Journal 2011)

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

Math Increasingly Central