Biophysical Simulations using QuickField

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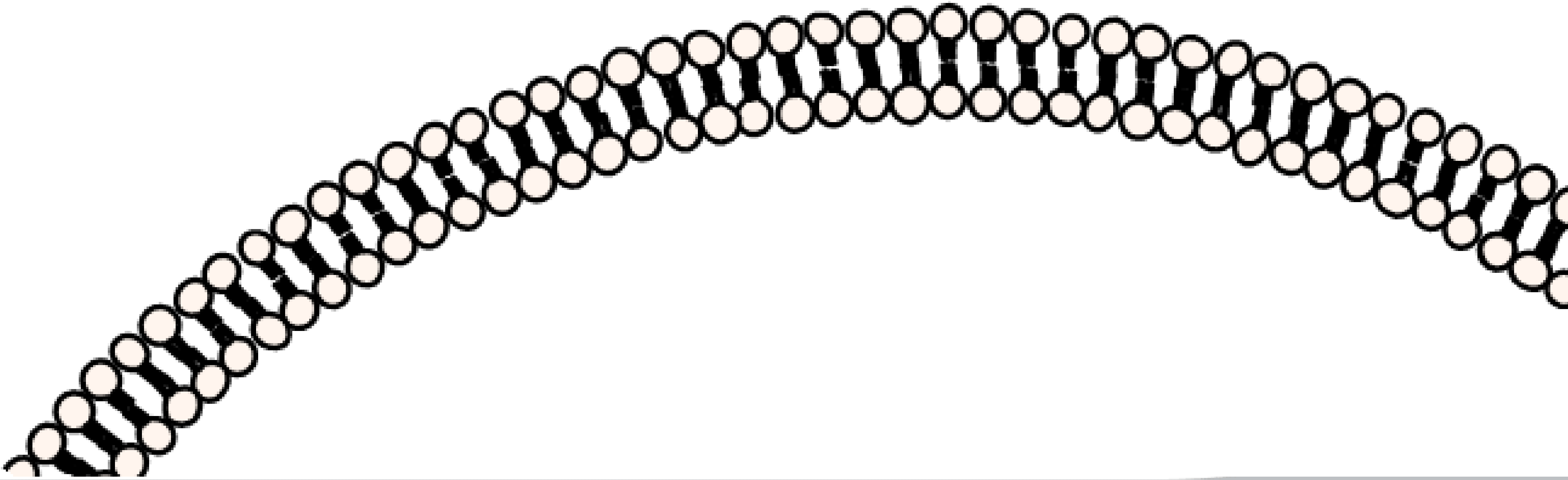
Biophysical Simulations using QuickField

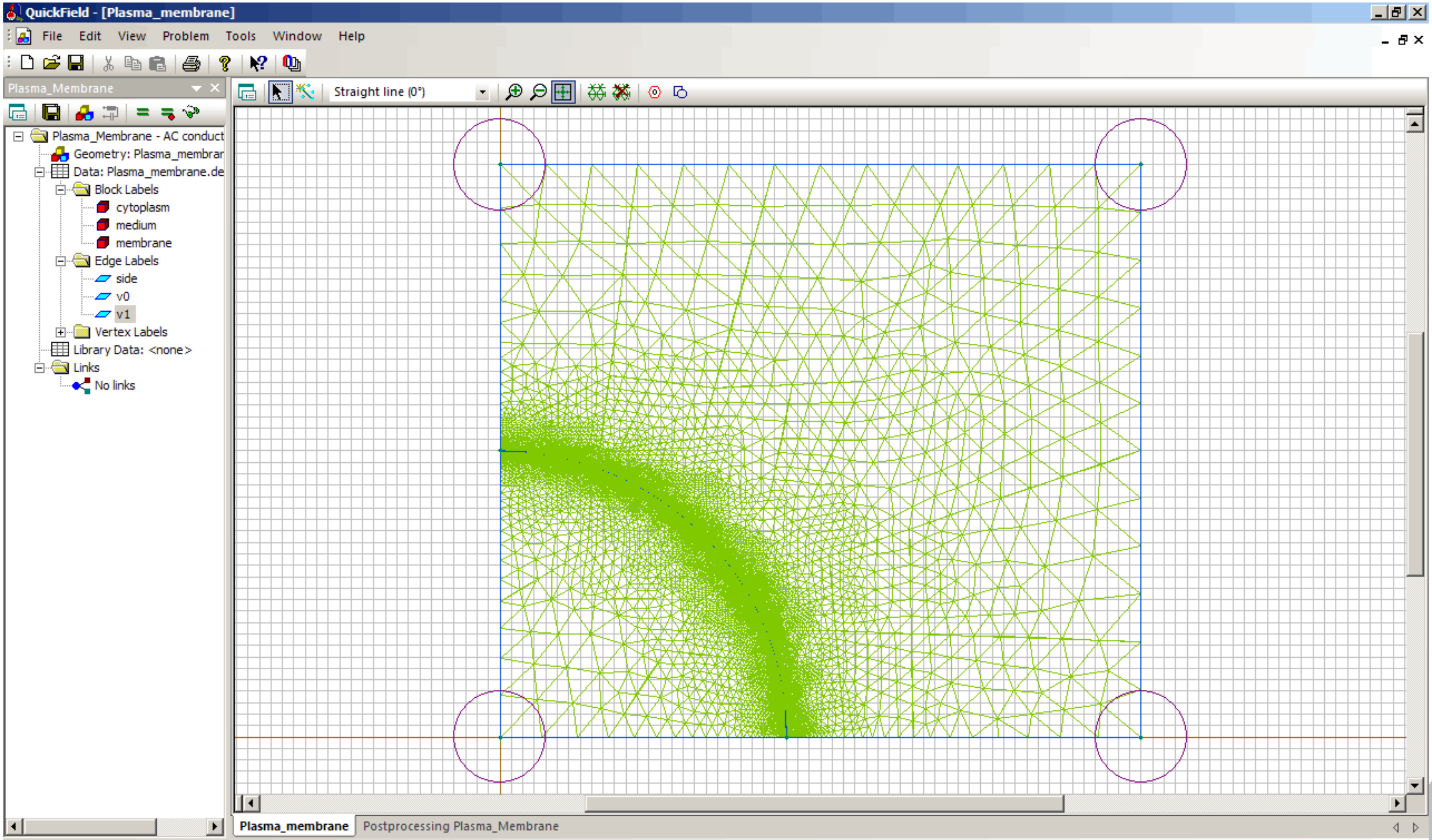
- Membrane and Cellular Size Scales
- Intrinsic Membrane Potentials
- Membrane Bound Charges
- Induced Membrane Potentials
  - External Plasma Membrane
  - Organelle Membranes
- Bioimpedance Simulations
- Dielectrophoresis Forces

Relative Size Scales

- Cells are ~50 micron size
- Membranes are ~ 7 nm in thickness
- Mesh density should span ~ 3 orders of magnitude

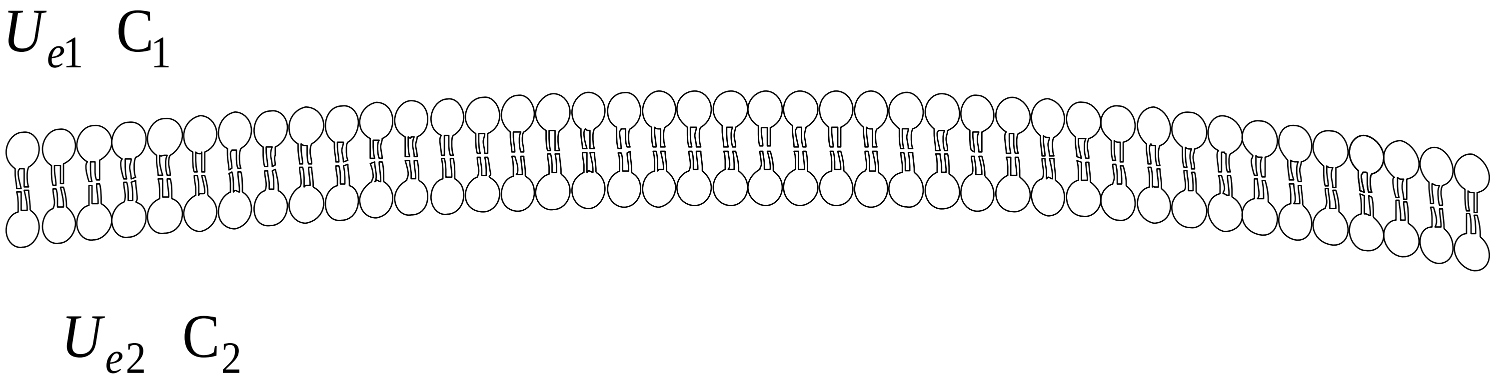


Scale modeling of biological membranes requires a hyperfine mesh density



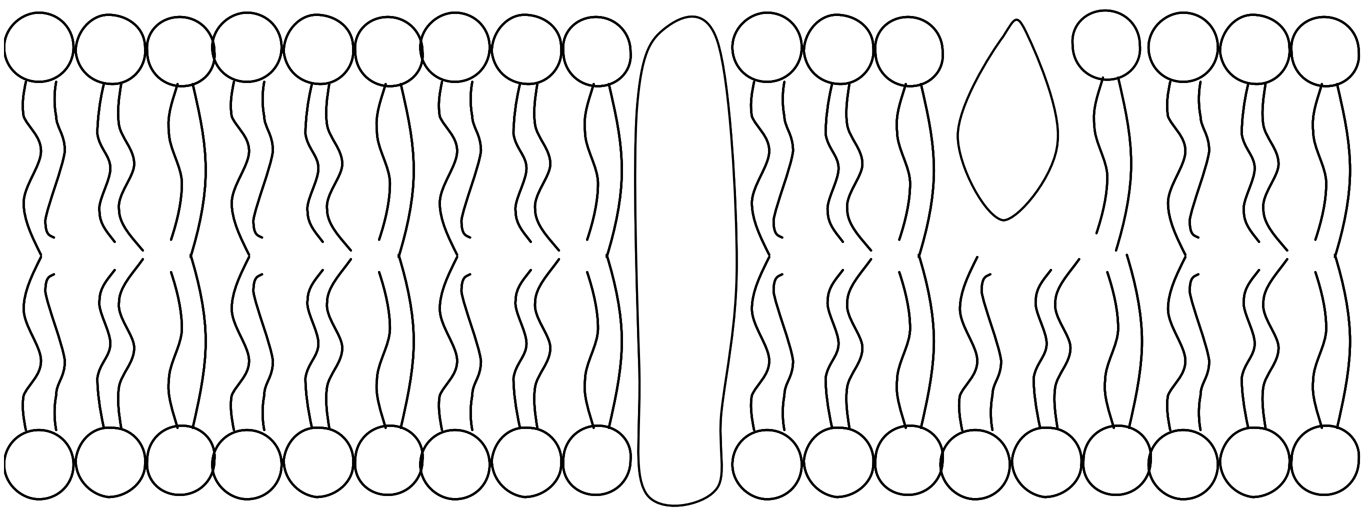
Membrane Potential

Membrane with ionic concentrations *C1* and *C2* on each side of the membrane.



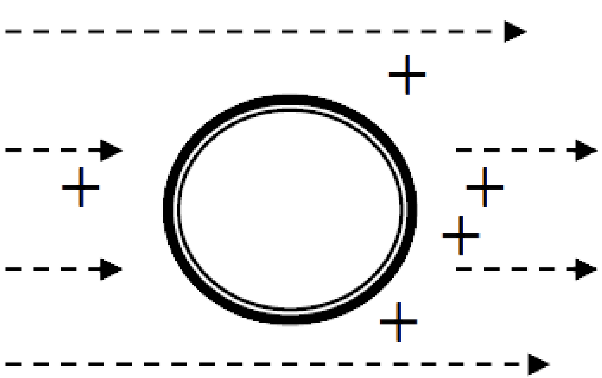
Membrane Charges

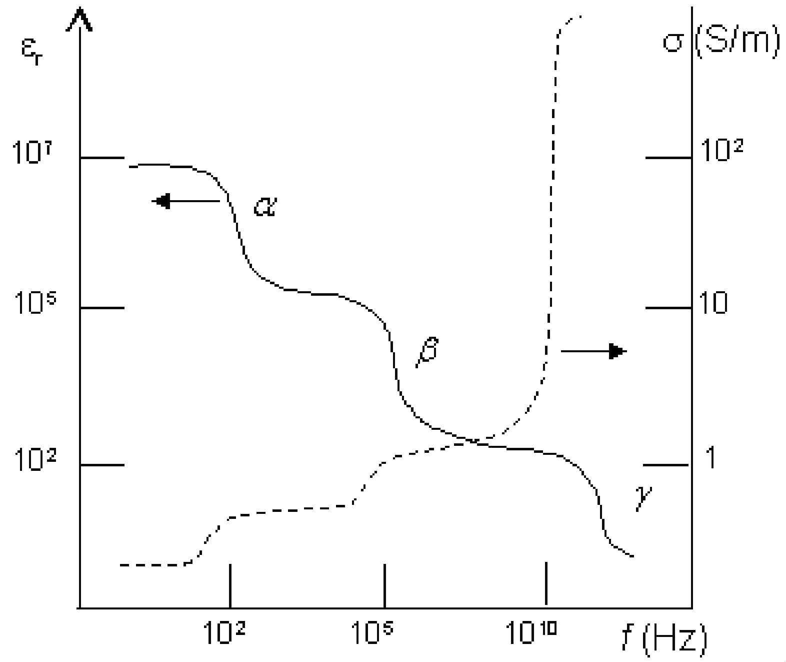
Section of plasma membrane with embedded membrane proteins. Cell membranes represent a boundary between living and nonliving matter on earth. The membrane encloses the cytoplasm containing organelles while remaining permeable to small molecules.



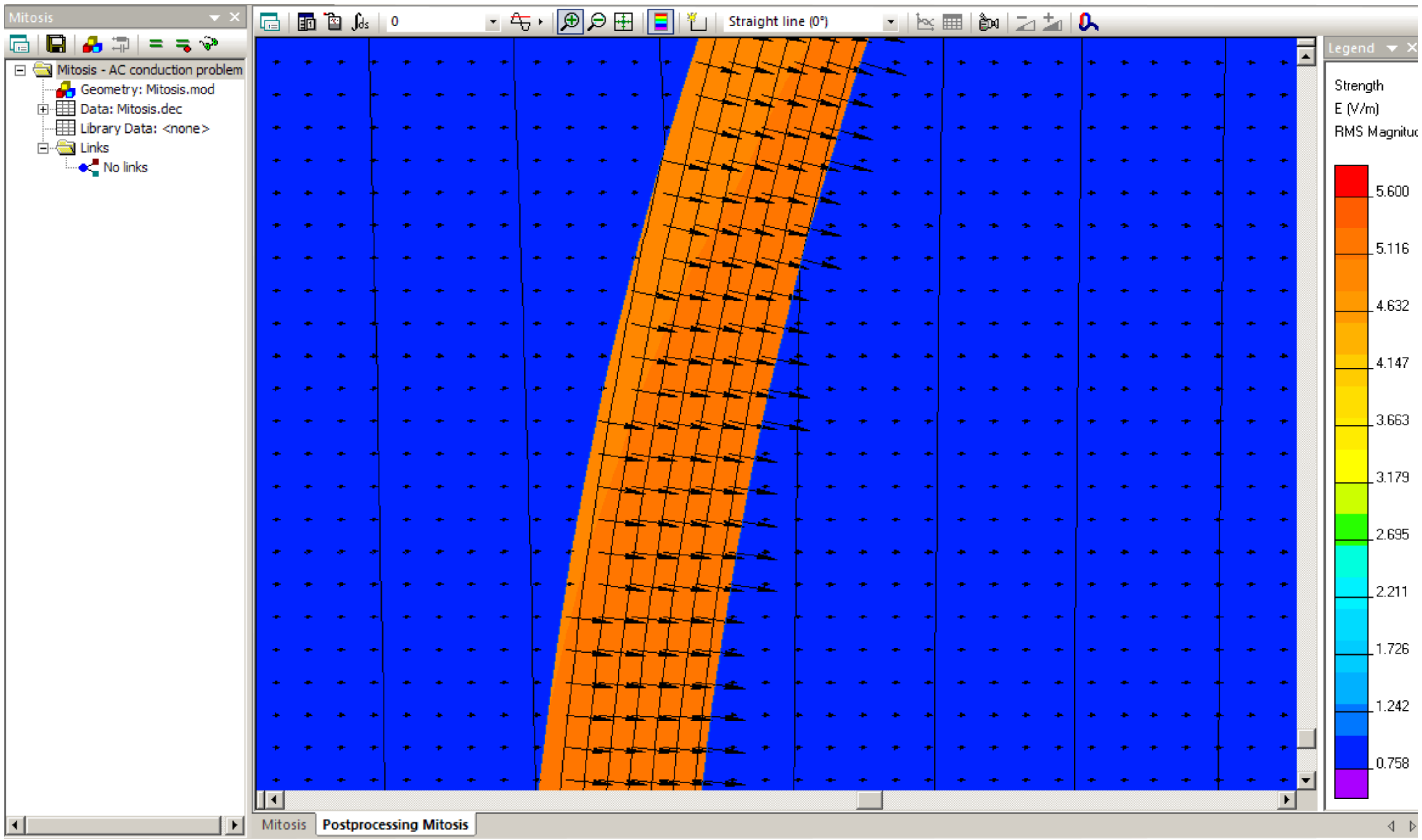
Modulation of membrane potential by external fields

- Motion of counter ions (α –frequency range below kHz)
- Maxwell-Wagner effect – potential differences developed across regions of differing permittivity





Amplification of E across the membrane



Bioimpedance Simulations

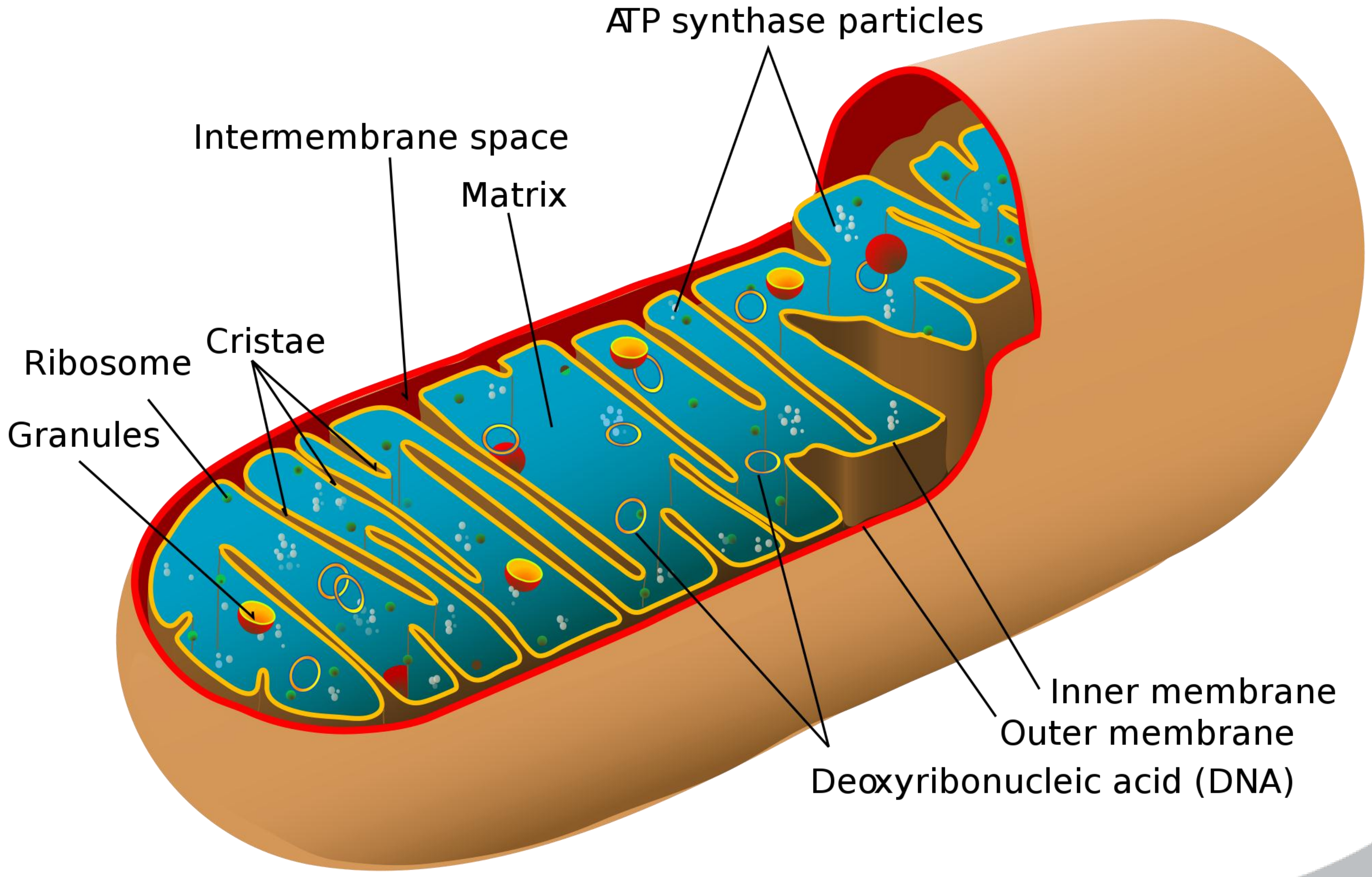
- Determine the effective σ and ε of tissue or cell suspension

$$J = \underbrace{\sigma E}_{J_{\text{active}}} + i\underbrace{\omega \varepsilon E}_{J_{\text{reactive}}}$$

$$\sigma = \frac{J_{\text{active}}}{E} \qquad \varepsilon = \frac{J_{\text{reactive}}}{E\omega}$$

Modeled using the AC Current Flow Module

Mitochondrion



Dielectrophoresis Force

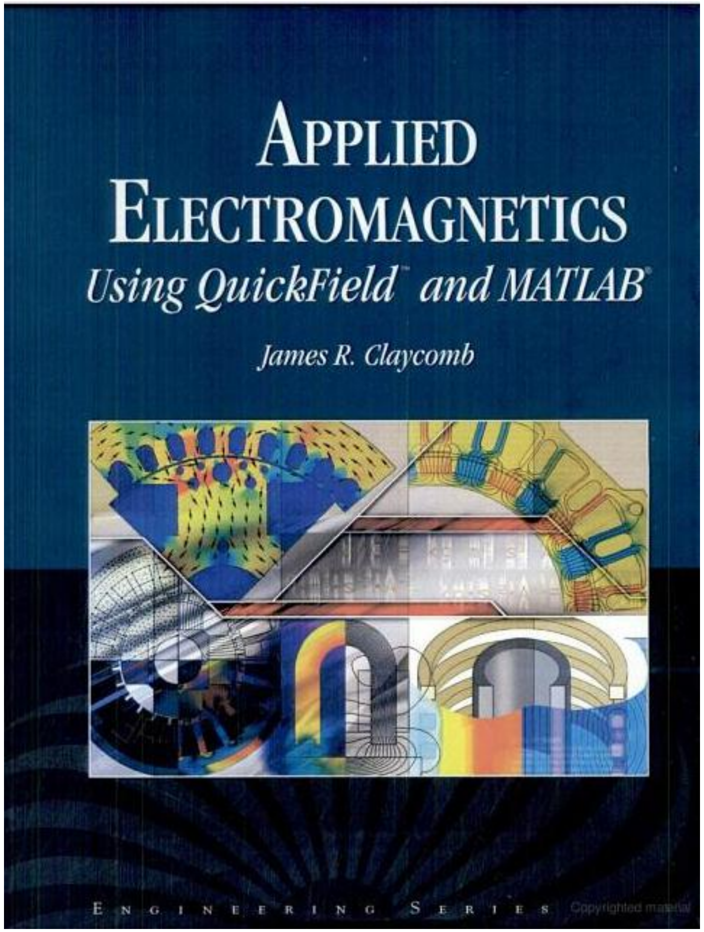
- Occurs in nonuniform fields, **F** = **p**·∇·**E**
- Direction of the force points towards or away from electric field gradient direction
- Direction depends on the relative permittivity of dielectric particles with respect to the medium
- Application to cell separation
- AC Fields

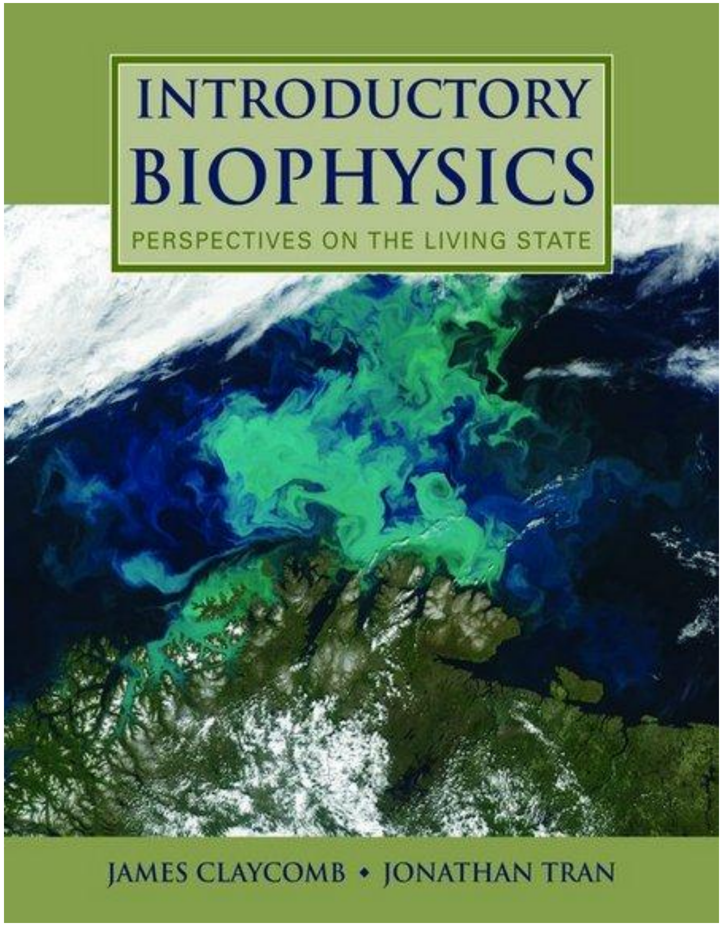
$$F = 2\pi r^3 \varepsilon_m \operatorname{Re}\left(\frac{\varepsilon_p^* - \varepsilon_m^*}{\varepsilon_p^* + 2\varepsilon_m^*} \right) \nabla E_{\text{rms}}^2$$

Key Points

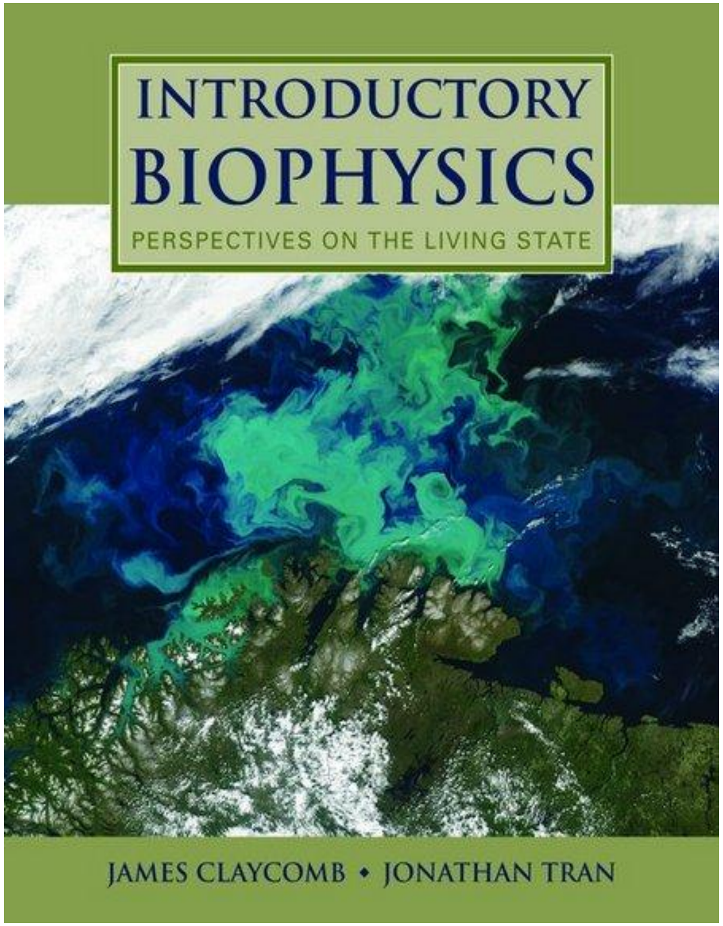
- Low frequency fields are screened from the interior of cells
- High frequency fields penetrate cells modulating the organelle potential differences
- External fields are amplified across cell membranes
- Dielectrophoresis force occurs in nonuniform fields and is either attractive or repulsive depending on the relative permeability of dielectric particles relative to their environment.

Books by Dr. James Claycomb:





Further Applications: Introductory Biophysics by Jones & Bartlett Learning



Analysis & Symmetry	Biophysical Calculations in QuickField
Electrostatic •X-Y Symmetry •Axial Symmetry	• Field distributions of molecular ion and dipole sources • Plasma and organelle membrane potentials and field distributions • Forces and torques on membrane bound protein dipole sources • Dielectrophoretic force acting on cells and biomolecules in nonuniform electric fields • Electrorotation forces on cells of various shapes.
Magnetostatic •X-Y Symmetry •Axial Symmetry	• Magnetic fields generated by bioelectric currents • Magnetotactic bacteria • Current dipole model of action potentials • Forces and torques acting between bioelectric current sources • Forces and torques acting on bioelectric sources in external B fields • Magnetostatic forces acting on weakly diamagnetic biomaterials in high magnetic fields
AC Magnetic •X-Y Symmetry •Axial Symmetry	• AC currents induced in tissue and cells by alternating magnetic fields • Joule heating of tissue by alternating magnetic fields • AC currents and induced potentials across plasma and organelle membranes
Transient Magnetic •X-Y Symmetry •Axial Symmetry	• Transient currents induced in biomaterials by magnetic field pulses and periodic waveforms (including square wave, triangle, saw tooth, rectified sine wave, delta train) • Transient currents and induced potentials across plasma and organelle membranes

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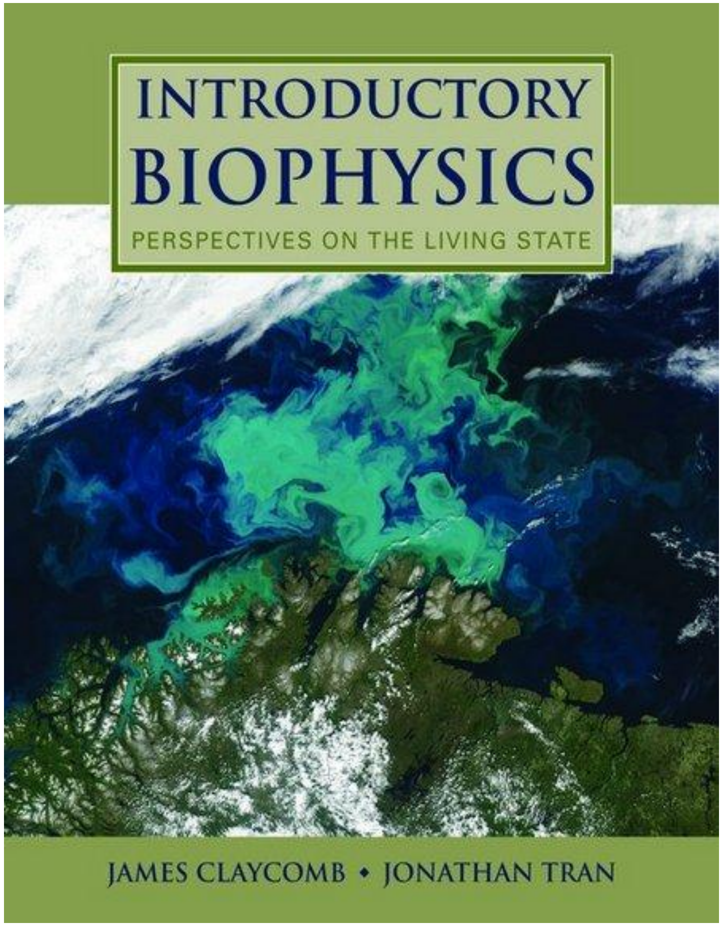

DC Conduction •X-Y Symmetry •Axial Symmetry	• DC current flow through biomaterials • Bioelectric return currents due to action potentials • DC currents through gap junctions, plasma and organelle membranes
AC Conduction •X-Y Symmetry •Axial Symmetry	• Bioimpedance calculations of tissue and cells • AC currents induced in tissue and cells by alternating magnetic fields
Thermal •X-Y Symmetry •Axial Symmetry	• Heat transfer between biomaterials via radiation, convection and conduction
Stress •X-Y Symmetry •Axial Symmetry	• Stresses and strains in biomaterials with specified Young's modulus and Poisson's ratio •Coupled electric stresses in biomaterials •Coupled thermal stresses in biomaterials
Circuit Analysis (AC Magnetics and Transient Magnetics)	• Equivalent circuit models of cells and tissue under electrical stimulation • Dendrite passive signal propagation • Gap junction circuit models • Circuit models of electrode interfaces • Electrical circuits linked to tissue elements constructed in AC and Transient Magnetics Modules