جامعة الملك عبدالله للعلوم والتقنية
King Abdullah University of Science and Technology

Information Technology
Research Computing

Parallèles Oct 4th/5th 2016
by Alain Clò

http://researchcomputing.kaust.edu.sa

- Parallèles
- 4-5 Oct 2016
- 9am-4pm
- In Library Sea View Room

http://researchcomputing.kaust.edu.sa

Agenda :

June 14th

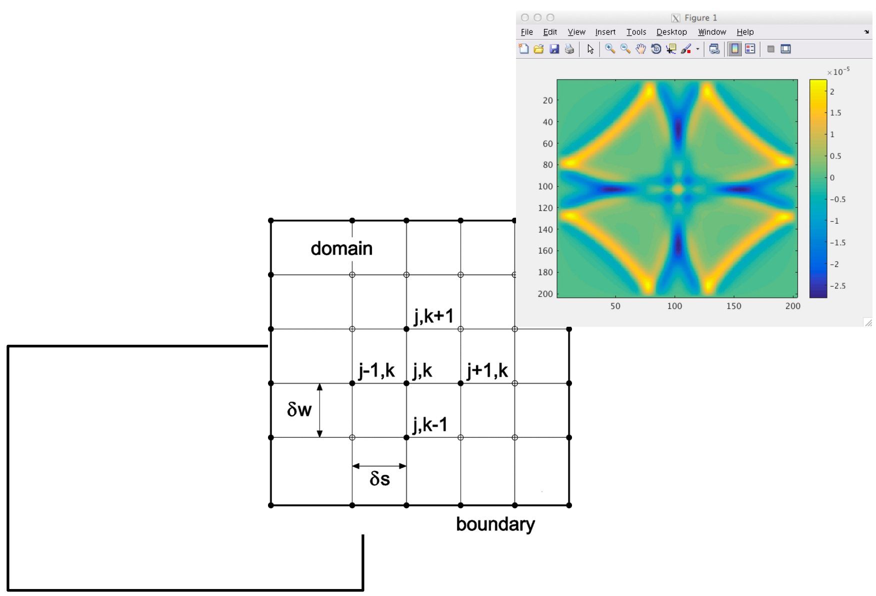
09:00-12:00 : Intro-Physics-Waves-Maths

14:00-16:00 : Numerical Methods-Discretisation

June 15th

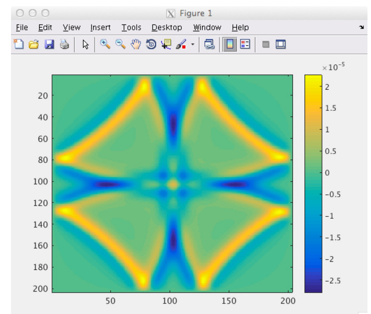
09:00-12:00 : Acoustic 2D

14:00-16:00 : Acoustic 2D

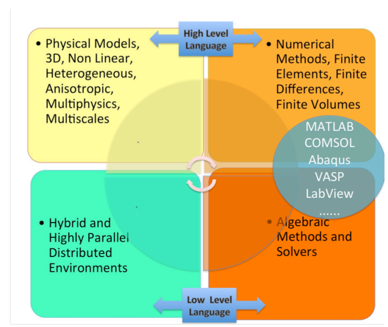


Parallèles - Introduction

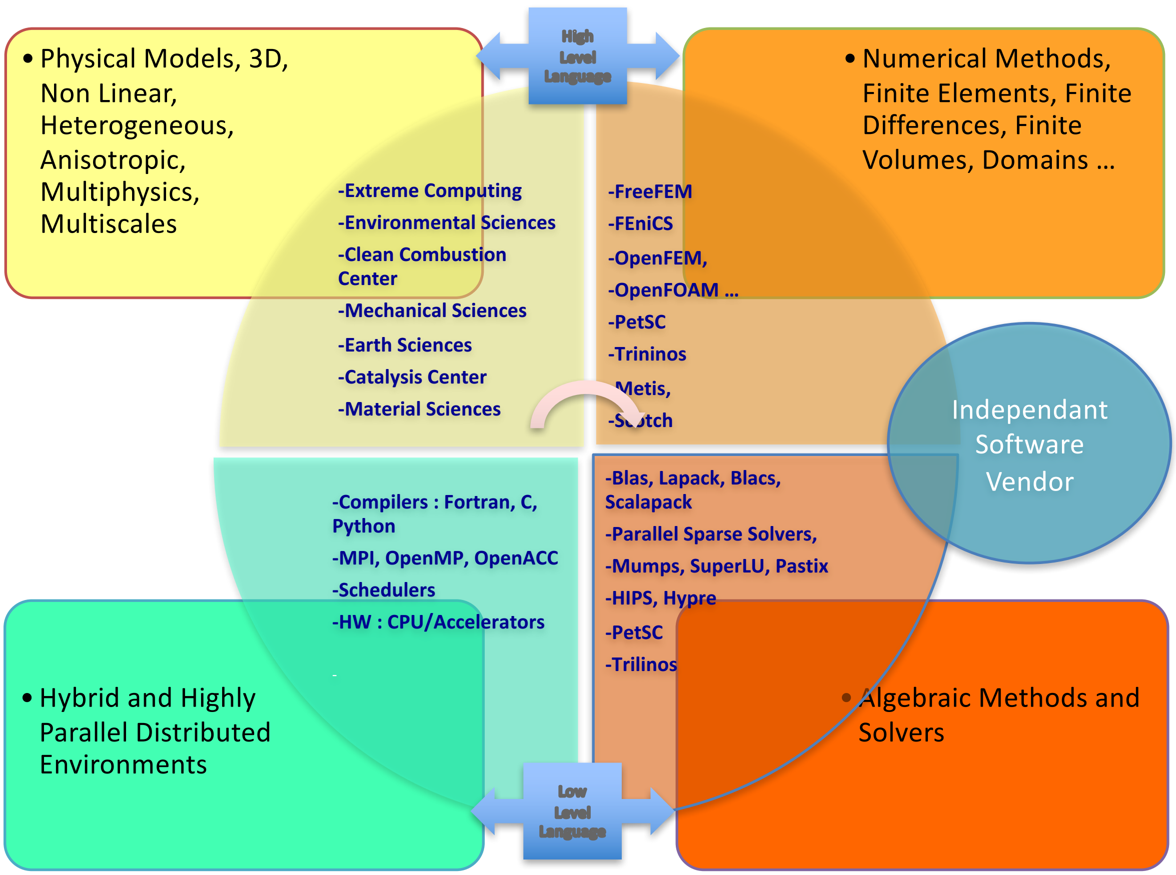
- This workshop is meant for sharing practice in scientific computing and high performance and scientific computing and spans wide interests and encourage creation and innovation.



- Physics
- Maths, Applied Maths
- Programming
- Systems

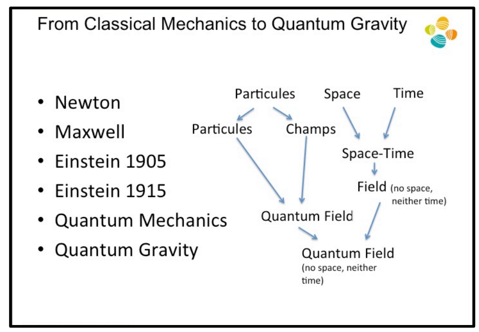


Scientific Computing Architecture OpenSource and ISV Software

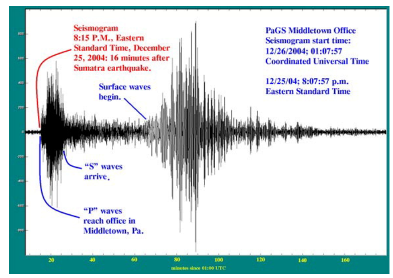


Physics

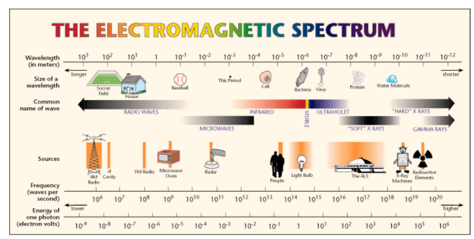
- From Classic Mechanics to Quantum Gravity
- Laws of Conversation
- Thermodynamics
- From Conservation Laws to Wave Equation
- Some other classic problems

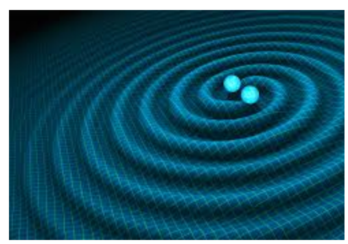


Waves



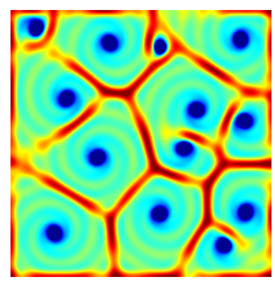
- What is a wave
- Types of waves
  - Acoustic
  - Elastic
  - Electromagnetic
  - Gravity
- Acoustic waves



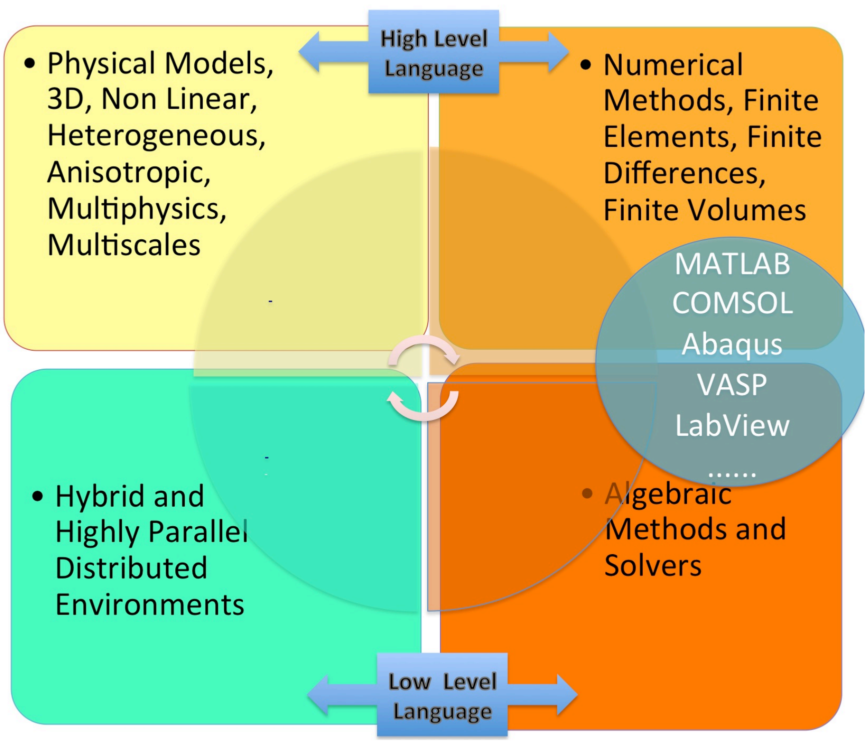


Mathematics

- Ordinary Differential Equations
- Partial Differential Equations
- Classification of second order Partial Differential Equations



Numerical Schemes



Explicit and Implicit Methods

- Explicit scheme:

$$Y(t+\Delta t) = F(Y(t))$$

- Implicit scheme:

$$G(Y(t), Y(t+\Delta t)) = 0$$

Aim: Find $Y(t+\Delta t)$

More afford necessary for implicit scheme.

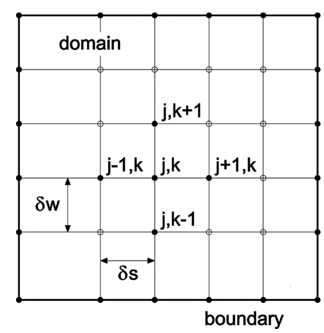
8

- Numerical Schemes
- Finite Difference
- Finite Elements
- Finite Volumes
- Integral Equations
- Spectral Methods

Discretisation

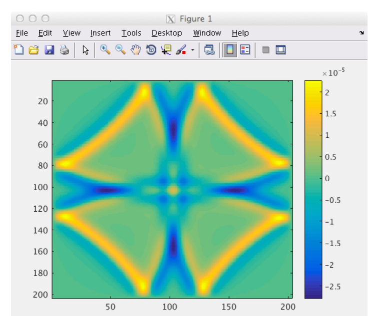
- Taylor Series
- Finite Differences
- Finite Elements
- Let's try to discretise with the wave equation

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n$$



Acoustic2D

- Wave equation
- Discretisation by finite difference in space and in time
- Algorithm
- coding Acoustic2D
  - Fortran
  - Matlab
  - Python
  - Julia
- Parallelisation



Thank You

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Physics

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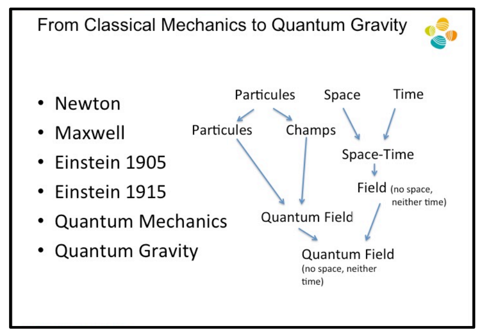
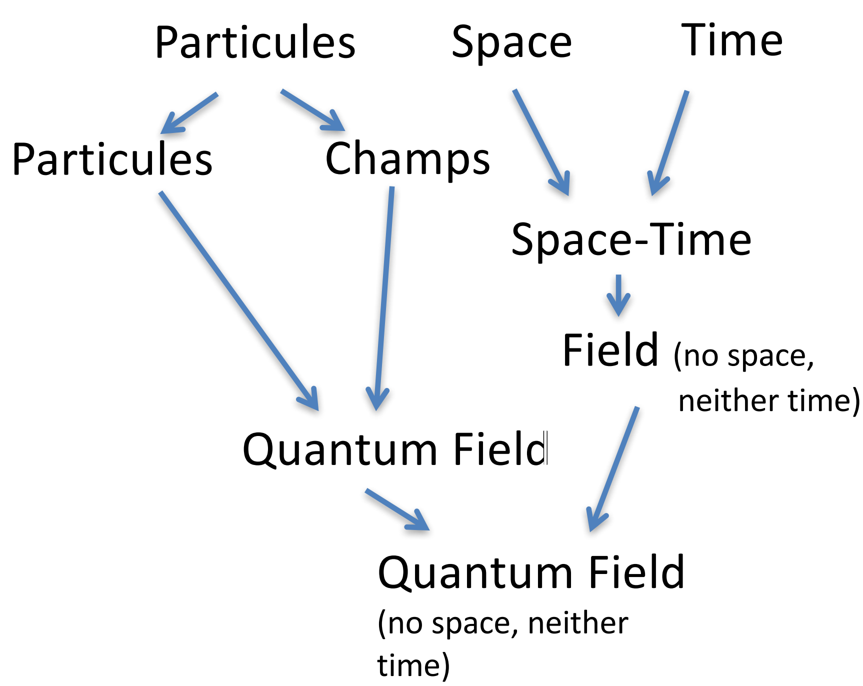
- From Conservation Laws to Wave Equation
- Some other classic problems



From Classical Mechanics to Quantum Gravity

- Democrite
- Newton
- Maxwell
- Einstein 1905
- Einstein 1915
- Quantum Mechanics
- Quantum Gravity



Thermodynamics Principles

- Heat and Temperature in relation with Energy and Work
- Principles
  - 1 Energy Conservation
  - 2 Entropy - Irreversibility
  - 3 Residual Entropy

Boltzmann $S = k \log W$

Triumph of Classical Physics: The Conservation Laws

- Conservation of energy: The total sum of energy (in all its forms) is conserved in all interactions.
- Conservation of linear momentum: In the absence of external forces, linear momentum is conserved in all interactions.
- Conservation of angular momentum: In the absence of external torque, angular momentum is conserved in all interactions.
- Conservation of charge: Electric charge is conserved in all interactions.

Continuity Equation

- Describes the transport of a quantity that can be a mass, an energy, a momentum, an electric charge, a probability
- Stronger, local form of conservation laws
  - Conservation of mass $\frac{\partial \rho}{\partial t} + \nabla . \rho \vec{v} = 0$
  - Conservation of energy $\frac{\partial u}{\partial t} + \nabla . \vec{q} = f$
  - Conservation of momentum linear $\rho \frac{\partial u}{\partial t} + \frac{\partial P}{\partial x} = 0$
  - Conservation of electric charge $\frac{\partial \rho}{\partial t} + \nabla . \vec{J} = 0$
- Noether's Theorem : invariants with respect to time, space and orientation translations.

The Laws of Thermodynamics

- **The “zeroth” law**: Two systems in thermal equilibrium with a third system are in thermal equilibrium with each other.
- **First law** = **Conservation of Energy** : The change in the internal energy ΔU of a system is equal to the heat Q added to a system minus the work W done by the system.
- **Second law** = **Irreversibility**. It is not possible to convert heat completely into work without some other change taking place.
- **Third law**: It is not possible to achieve an absolute zero temperature

Maxwell's Equations Local form

- Gauss' s law : $\nabla . \vec{E} = \rho_0 \,/\, \varepsilon_0$
  (*E* electric field)

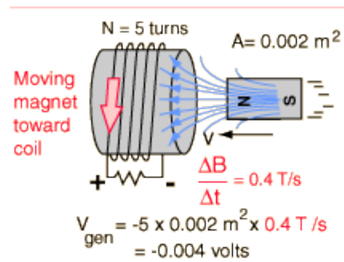
- Gauss' s law : $\nabla . \vec{H} = 0$
  (*H* magnetic field)

- Faraday' s law: $\nabla_{\wedge} \vec{E} = -\frac{\partial \vec{B}}{\partial t}$
  (*B* magnetic induction)

- Ampère' s law: $\nabla_{\wedge} \vec{B} = \mu_0 \vec{J} + \varepsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t}$
  (*J* courant density)

Maxwell's Equations Integral/Weak Form

- Gauss' s law (Φ_E): $\oint \vec{E} \cdot d\vec{A} = \frac{q}{\varepsilon_0}$
  (electric field)
- Gauss' s law (Φ_B): $\oint \vec{B} \cdot d\vec{A} = 0$
  (magnetic field)
- Faraday' s law: $\oint \vec{E} \cdot d\vec{s} = -\frac{d\Phi_B}{dt}$



- Ampère' s law: $\oint \vec{B} \cdot d\vec{s} = \mu_0 \varepsilon_0 \frac{d\Phi_E}{dt} + \mu_0 I$

Conversation Laws

- Conservation of mass $\frac{\partial \rho}{\partial t} + \nabla . \rho \vec{v} = 0$

  or Continuity Equation
- Conservation of energy $\frac{\partial u}{\partial t} + \nabla . \vec{q} = f$
- Conservation of momentum linear

$$\rho \frac{\partial u}{\partial t} + \frac{\partial P}{\partial x} = 0$$

- Conservation of electric charge $\frac{\partial \rho}{\partial t} + \nabla . \vec{J} = 0$

From Maxwell equations to the Electromagnetic Wave Equation

- Constitutive Law $\vec{B} = \mu\vec{H}; \vec{D} = \varepsilon\vec{E}$
- Maxwell-Faraday $\nabla_\wedge\vec{E} = -\frac{\partial\vec{B}}{\partial t}$

$$\nabla_\wedge\vec{E} = -\mu\frac{\partial\vec{H}}{\partial t} \quad => \quad \nabla_\wedge\nabla_\wedge\vec{E} = -\mu\frac{\partial\,\nabla_\wedge\vec{H}}{\partial t}$$

- Maxwell-Ampere

$$-\nabla^2\vec{E} = -\mu\frac{\partial}{\partial t}(\frac{\partial\vec{D}}{\partial t} + \vec{J}) \quad \& \quad \vec{J} = 0$$

- Wave Equation $\frac{\partial^2\vec{E}}{\partial t^2} = \frac{1}{\varepsilon_0\mu_0}\Delta\vec{E}$

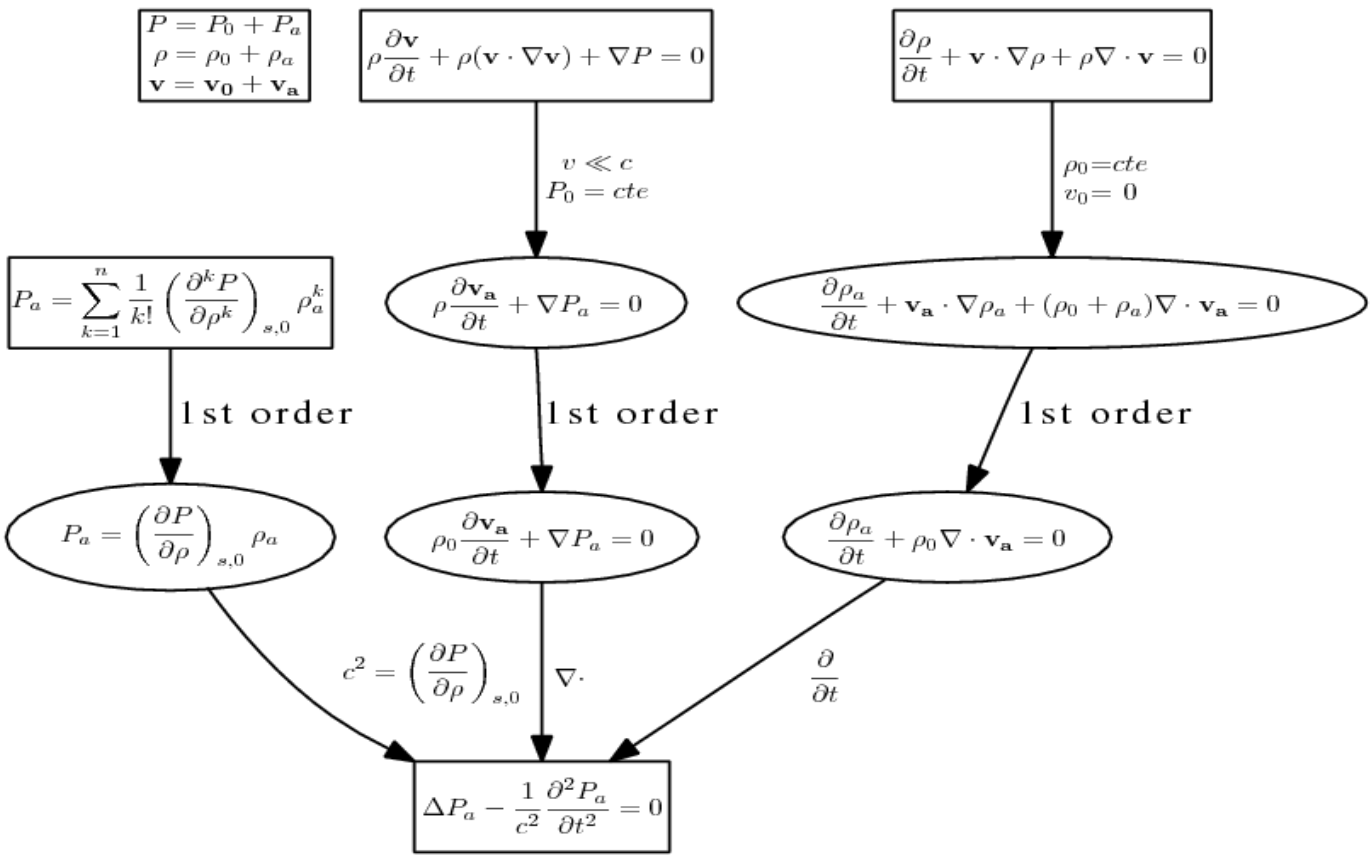
From Newton Equation to the Elastic Wave Equation

- Constitutive Law (Hooke)
  - $\sigma = C\varepsilon(\vec{u});$
- Lamé Coefficients
  - $\sigma = \lambda \mathrm{Tr}(\varepsilon)\mathrm{I} + 2\mu\varepsilon;\ d = \nabla.\,\vec{u};\ r = \nabla_{\wedge}\,\vec{u}$
- Dynamic Equation $\quad \dfrac{\partial^2 \vec{u}}{\partial t^2} - \nabla \cdot \sigma = \rho \vec{g}$
- P waves : $C_p = \sqrt{\dfrac{\lambda + 2\mu}{\rho}} \quad \dfrac{\partial^2 \vec{d}}{\partial t^2} - \Delta d = \nabla.\,\vec{g}$
- S waves : $C_s = \sqrt{\dfrac{\mu}{\rho}} \quad \dfrac{\partial^2 \vec{r}}{\partial t^2} - \Delta r = \nabla_{\wedge}\vec{g}$

From Conservation Laws to the Acoustic Wave Equation

- State Equation or Constitutive Law $$PV = nRT$$
- Mass Conservation or Continuity Equation $$\frac{\partial \rho}{\partial t} + \nabla \rho v = 0$$
- Momentum Conservation $$\gamma = \frac{1}{\rho} \nabla \sigma + g$$
  or Euler Equation $$\rho \frac{\partial u}{\partial t} + \frac{\partial P}{\partial x} = 0$$
- Wave Equation $$\frac{\partial^2 P}{\partial t^2} = c^2 \Delta P$$

Derivation of the acoustic wave equation



Some other Classic Problems

- Heat Diffusion
  - Heat Equation $\frac{\partial u}{\partial t} - \alpha \Delta u = 0$
- Electromagnetic Potentials
  - Poisson, Laplace Equations $\nabla E = \frac{\rho}{\varepsilon};\ E = -\nabla V; \Delta V = 0$
- Quantum Mechanics
  - Schrödinger Equation $\frac{\partial \psi}{\partial t} - ih \frac{ih}{4m\pi} \Delta \psi = 0$

Questions and Type of Problems

- Equilibrium
- Steady State
- Boundary Value
- Time Dependent
- Transient
- Harmonic
- Well Posed

Thank You

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Waves

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- Types of waves
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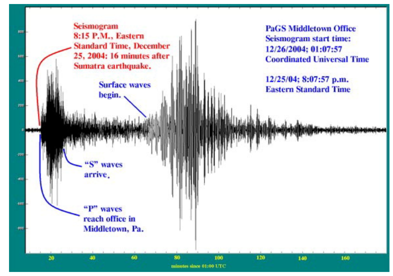
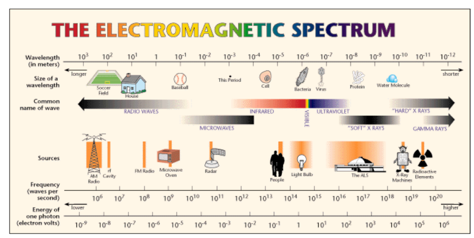
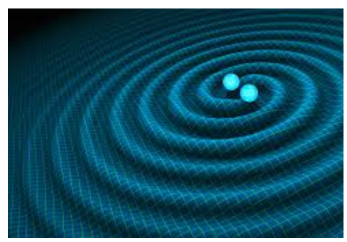
  - Gravity
- Acoustic waves

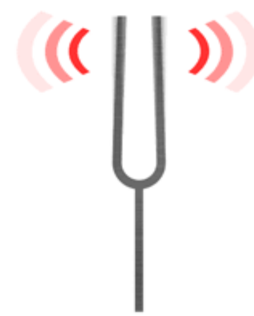


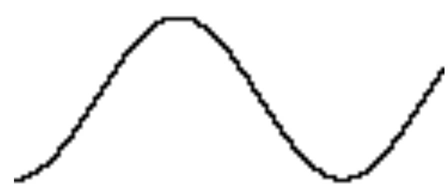




What are Waves?

Rhythmic disturbances that carry energy without carrying matter





Waves are everywhere in nature

- Sound waves,
- visible light waves,
- radio waves,
- microwaves,
- water waves,
- sine waves,
- telephone chord waves,
- stadium waves,
- earthquake waves,
- waves on a string,
- slinky waves

What is a wave?

- a wave is a disturbance that travels through a medium from one location to another.
- a wave is the motion of a disturbance

Types of Waves

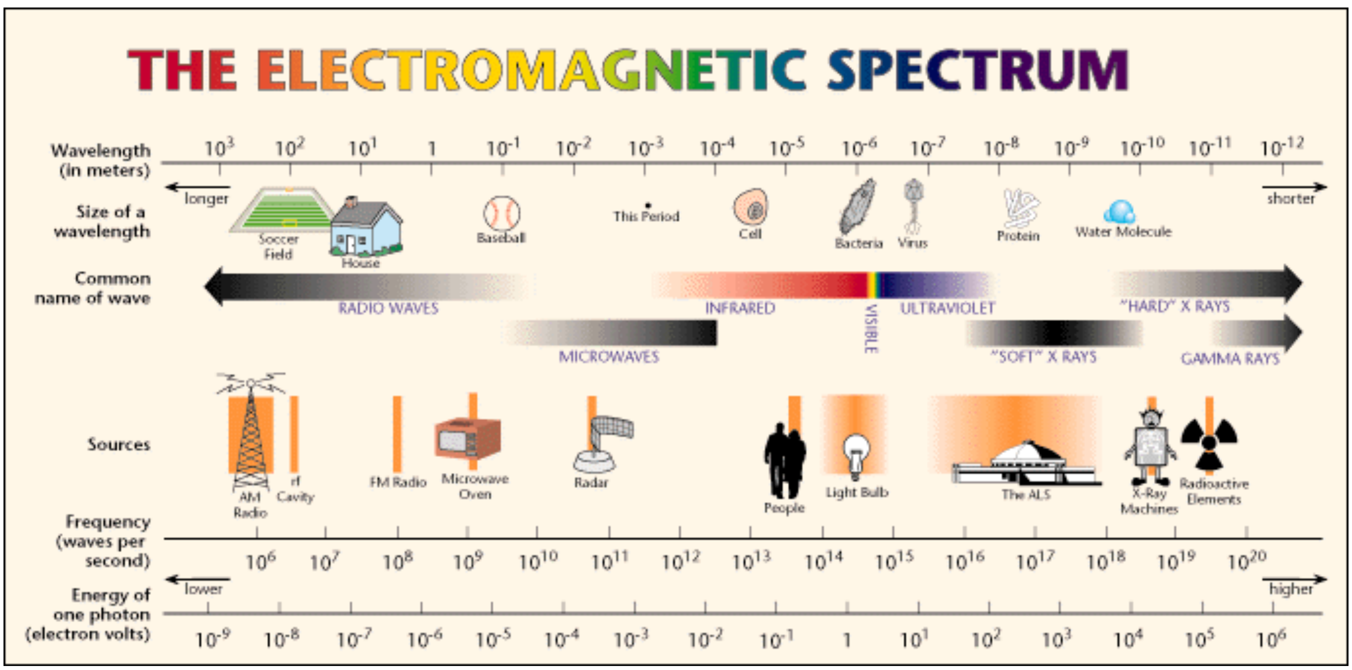
- Mechanical Waves – need matter (or medium) to transfer energy
  - Acoustic : medium is the substance through which a wave can travel in air, water, liquids, gases
  - Elastic : medium can be : particles, strings, solids
- Electromagnetic Waves – DO NOT NEED matter (or medium) to transfer energy
  - They do not need a medium, but they can go through matter (medium), such as air, water, and glass

Mechanical Waves

- Waves that need matter (medium) to transfer energy
  - Examples: Sound waves, ocean waves, ripples in water, earthquakes, wave of people at a sporting event

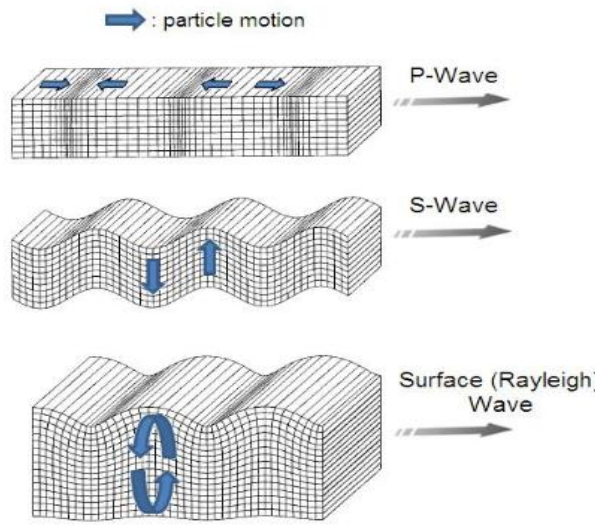
Electromagnetic Spectrum

The electromagnetic spectrum illustrates the range of wavelengths and frequencies of electromagnetic waves.



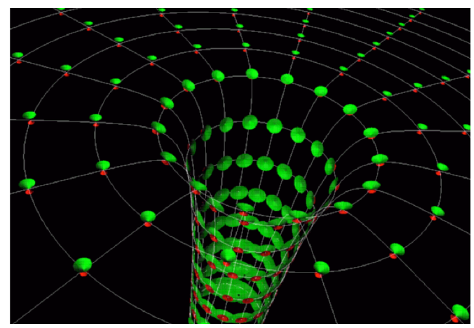
Seismic waves

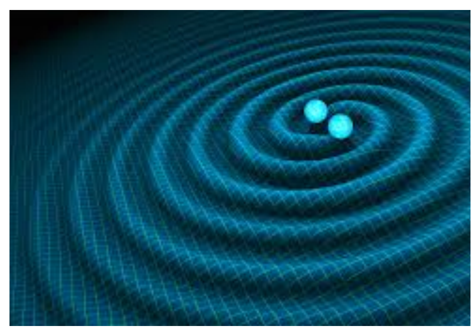
- Body waves
  - P compression, longitudinal
  - S shear, transverse
- Surface waves
  - Rayleigh
  - Love, transverse



Gravitational waves

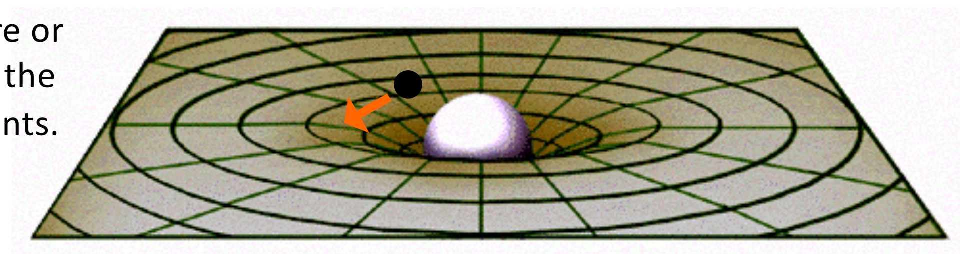
- $\{\Delta - \frac{\partial^2}{\partial t^2}\} h_{\mu\nu} = 0$
- Static gravitational fields are a curvature of space-time.
- A change in the gravitational field will generate a gravitational radiation – a wave of spacetime curvature.



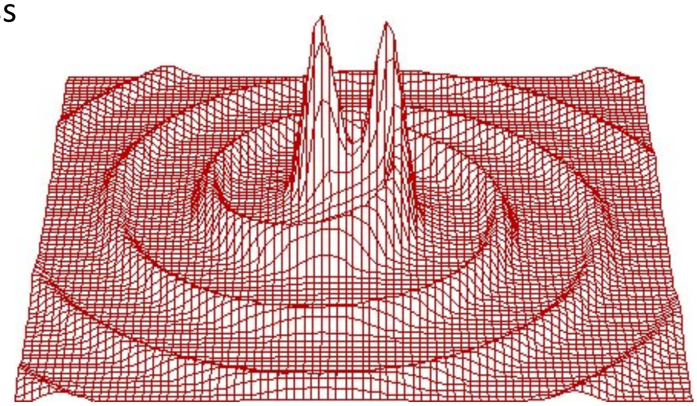


Gravitational Waves

Static gravitational fields are described in General Relativity as a curvature or warpage of space-time, changing the distance between space-time events.



Shortest straight-line path of a nearby test-mass is a ~Keplerian orbit.



If the source is moving
(at speeds close to c),
eg, because it's orbiting a companion, the "news" of the changing gravitational field propagates outward as gravitational radiation
a wave of spacetime curvature

Ultimate Goals for the Observation of GWs

- Tests of Relativity
  - Wave propagation speed (delays in arrival time of bursts)
  - Spin character of the radiation field (polarization of radiation from CW sources
  - Detailed tests of GR in P-P-N approximation (chirp waveforms)
  - Black holes & strong-field gravity (merger, ringdown of excited BH)

- Gravitational Wave Astronomy (observation, populations, properties)
  - Compact binary inspirals
  - Gravitational waves and gamma ray burst associations
  - Black hole formation
  - Supernovae in our galaxy
  - Newly formed neutron stars - spin down in the first year
  - Pulsars and rapidly rotating neutron stars
  - LMXBs
  - Stochastic background

Acoustic Waves

- Jean Rond de D’Alembert
- Joseph Fourier
- Hermann von Helmholtz
- Harry Nyquist
- Richard Courant-Friedrichs-Lewy

Jean Rond de d'Alembert

The general solution of the partial differential equation

$$\Box = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2.$$

is

where *f*(*x*-*ct*) represents a wave traveling in the forward (or positive) x-direction, and *f*(*x*+*ct*) represents a wave traveling in the negative x-direction.

Fourier

- A sum of plane waves are natural solution of the wave equation

- A plane wave
- Dispersion Relation
- The wave is defined by its pulsation ω, wavelength λ, wavenumber k and frequency f and period T.

Helmholtz

- In the Harmonic – Frequency domain
- The wave equation becomes

Helmholtz equation :

$$-c^2\Delta u - \omega^2 u = 0$$

$$-\Delta u - \ k^2 u = 0$$

pulsation w, wavelength l, wavenumber k and frequency f and period T

Dispersion

The scalar wave equation is verified by the vibration u(t,x)

Homogeneous medium

The wave solution is u(x,t)=F(x+ct)+G(x-ct) whatever are F and G (to be checked)

The wave is defined by pulsation ω, wavelength λ, wavenumber k and frequency f and period T. We have the following relations

A plane wave is defined by with the dispersion relation

The phase velocity is for any frequency

If the pulsation ω depends on k, we have and the group velocity is

which is identical to phase velocity for non-dispersive waves

Numerical Anisotropy and Dispersion

- CFL Condition - stability
  - $\Delta t << \frac{\Delta x}{\mathrm{c}}$, c velocity in the domain
- Nyquist Condition - accuracy
  - $\Delta t << \frac{2\pi}{\omega}$, ω frequency of the source

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Mathematics

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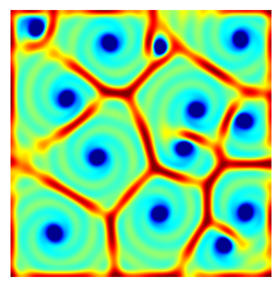
- Partial Differential Equations
- Classification of second order Partial Differential Equations



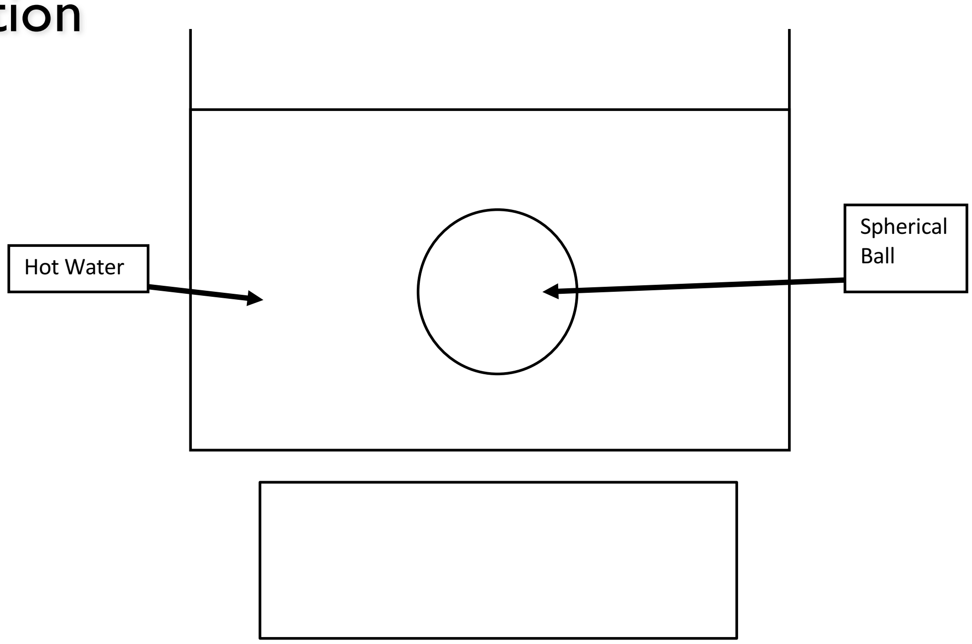
What is a Partial Differential Equation ?

- Ordinary Differential Equations have only one independent variable

- Partial Differential Equations have more than one independent variable

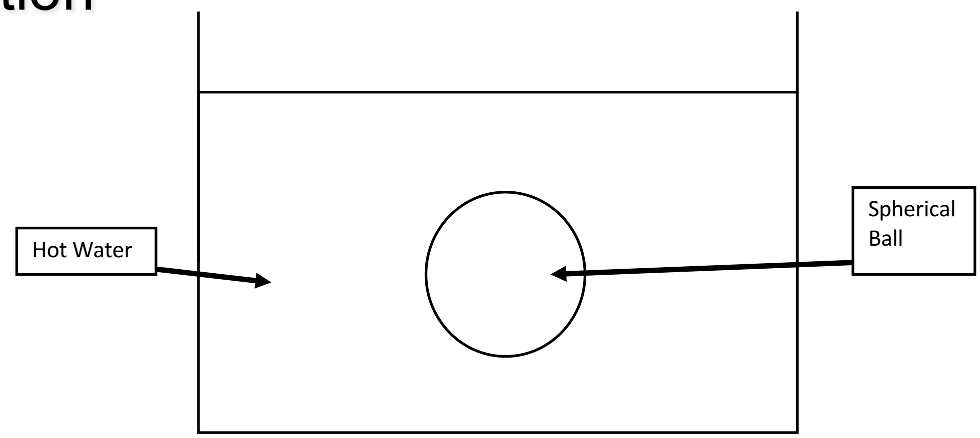
Subject to certain conditions: where *u* is the dependent variable, and *x* and *y* are the independent variables.

Example of an Ordinary Differential Equation



- Assumption: Ball is a lumped system.
- Number of Independent variables: One (t)

Example of an Partial Differential Equation



- Assumption: Ball is not a lumped system.
- Number of Independent variables: Four (r,θ,ϕ,t)

Classification of 2nd Order Linear PDE's

- where are functions of
- and is a function of

Classification of 2nd Order Linear PDE's

- Consider
  - if > 0 then the equation is Elliptic
  - if = 0 then the equation is Parabolic
  - if < 0 then the equation is Hyperbolic

Classification of 2nd Order Linear PDE's

- Elliptic Equation
  - Laplace equation for Steady State or Static Problems such as Electrostatic, Thermal Static, Potential Flow.
- Parabolic Equation
  - Heat equation for diffusion of heat, neutrons, chemicals, viscous flow. Dynamic. Non reversible. Infinite speed propagation.
- Hyperbolic Equation
  - Wave equation for acoustic, electromagnetism, elastodynamic. Dynamic. Reversible, Energy Conservation. Finite speed propagation.

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