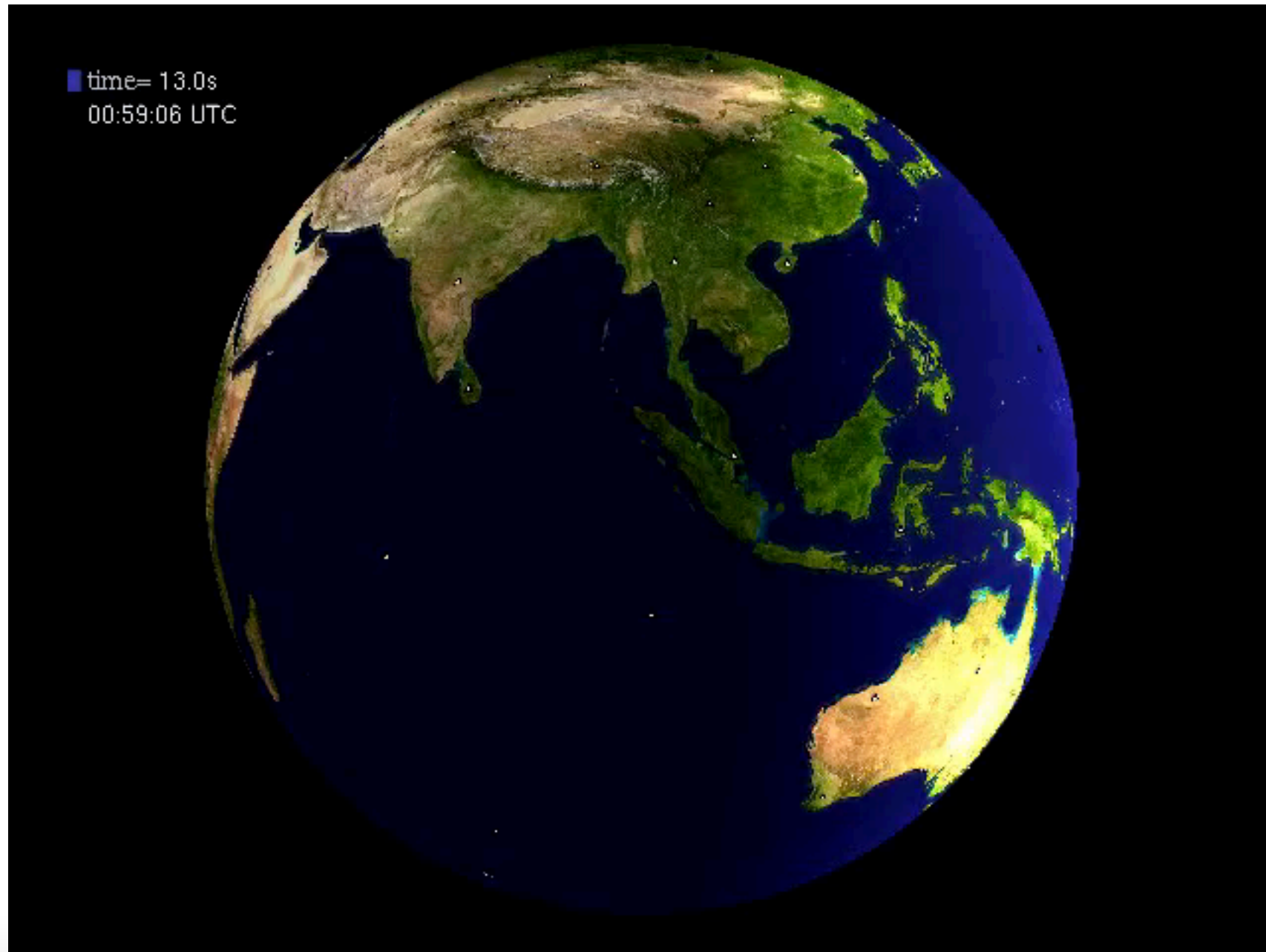


# Computational Geophysics

## ErSE 390C



# Computational Geophysics - ErSE 390C

Fall Semester 2016

## **Schedule:** (tentative)

week 1 Introduction to conservation laws for heat flow and wave propagation

week 2 Finite-differences method for heat flow

week 3 Finite-differences method for wave propagation

- No classes - Eid Al-Adha break

week 4 Higher-order Finite-differences method for tsunami waves

week 5 Introduction to Pseudo-spectral method

week 6 Pseudo-spectral method for wave propagation

week 7 Introduction to Finite-element method

week 8 Finite-element method for steady-state heat flow

week 9 Finite-element method for unsteady-state heat flow

week 10 Introduction to spectral-element method

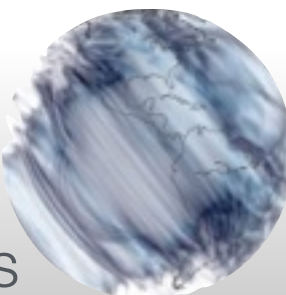
- No classes - semester break

week 11 Spectral-element method for heat flow

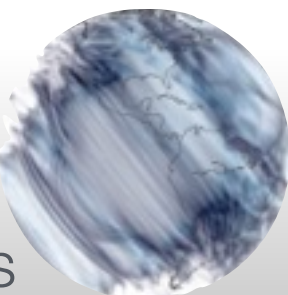
week 12 Spectral-element method for 1D wave propagation

week 13 Spectral-element method for 2D elastic wave propagation

week 14 Spectral-element method for 3D viscoelastic wave propagation



# Pseudo-spectral methods







# Galactic dynamics





# Boltzmann equation

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$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla f + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{p}} = \left( \frac{\partial f}{\partial t} \right)_{\text{coll}}$$

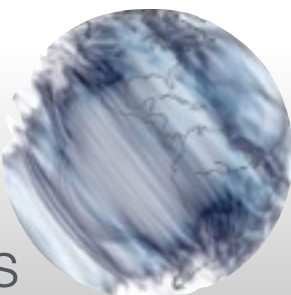
**F** Force field

*f* probability density function

**p** momentum

*m* particle mass

describes statistical behaviour of a thermodynamic system in non-equilibrium state



Quantum theory

optimized structure for  
organic molecules  
based on Density Functional  
Theory (DFT)



# Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left[ \frac{-\hbar^2}{2\mu} \nabla^2 + V(\mathbf{r}, t) \right] \Psi(\mathbf{r}, t)$$

$\hbar$  Planck constant

$\Psi$  wave function

$V$  potential energy

$\mu$  “reduced” particle mass

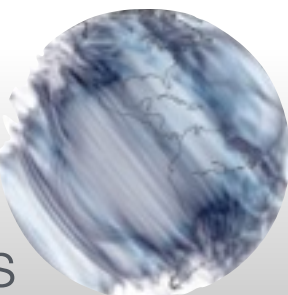
describes quantum state of a quantum system with time  
(single non-relativistic particle)





Fluid dynamics

Computational Geophysics





# Navier-Stokes equation

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$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \mathbf{u}$$

$P$  pressure field

$\mathbf{u}$  flow velocity vector

$\nu$  viscosity

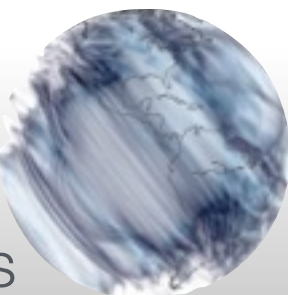
$\rho$  density

describes force balance within a fluid





# Wave propagation



# 1D wave equation

2nd-order partial differential equation:

$$\rho(x)\partial_t^2 u(x, t) = \partial_x[\kappa(x)\partial_x u(x, t)], \quad (x \in [0, L], t \in [0, +\infty))$$

## velocity-stress formulation

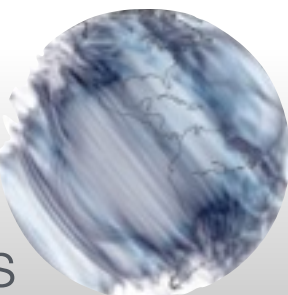
1st-order partial differential equations

$$\rho(x)\partial_t v(x, t) = \partial_x T(x, t)$$

$$\partial_t T(x, t) = \kappa(x)\partial_x v(x, t)$$

$$v(x, t) = \partial_t u(x, t)$$

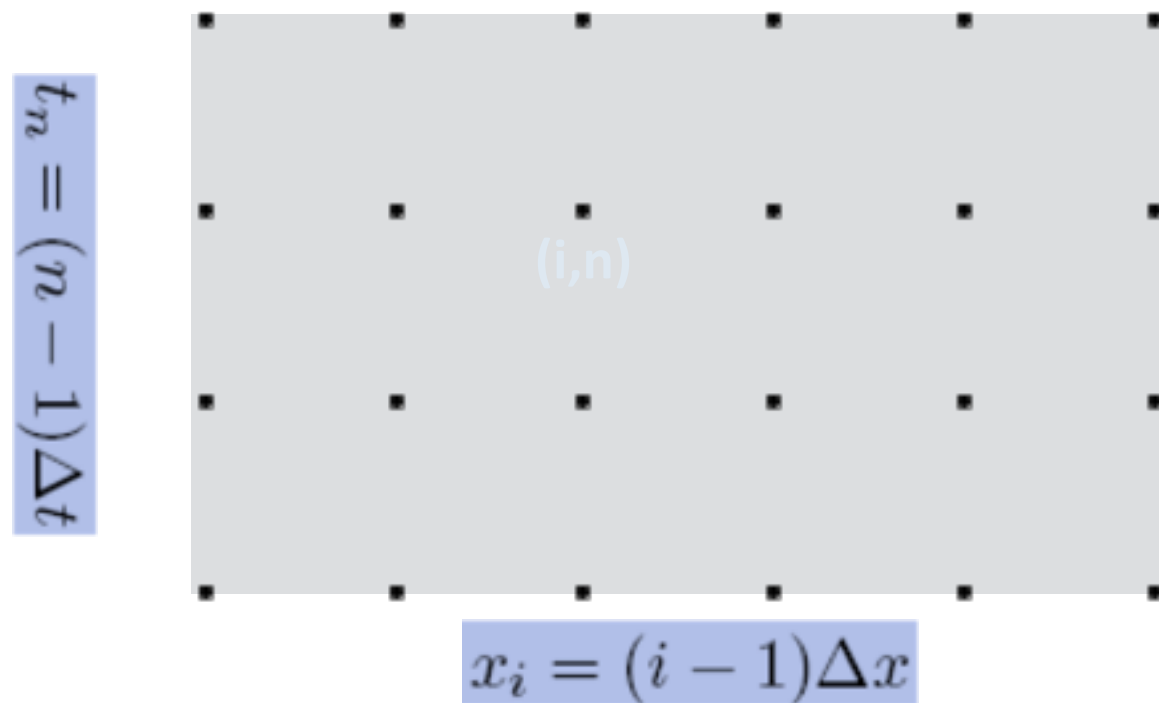
$$T(x, t) = \kappa(x)\partial_x u(x, t)$$





# Pseudo-spectral method

**Discretization**  $u_i^n = u(x_i, t_n)$



continuous form:

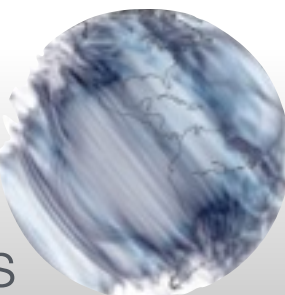
$$\rho(x)\partial_t v(x, t) = \partial_x T(x, t)$$

$$\partial_t T(x, t) = \kappa(x)\partial_x v(x, t)$$

discretized form:

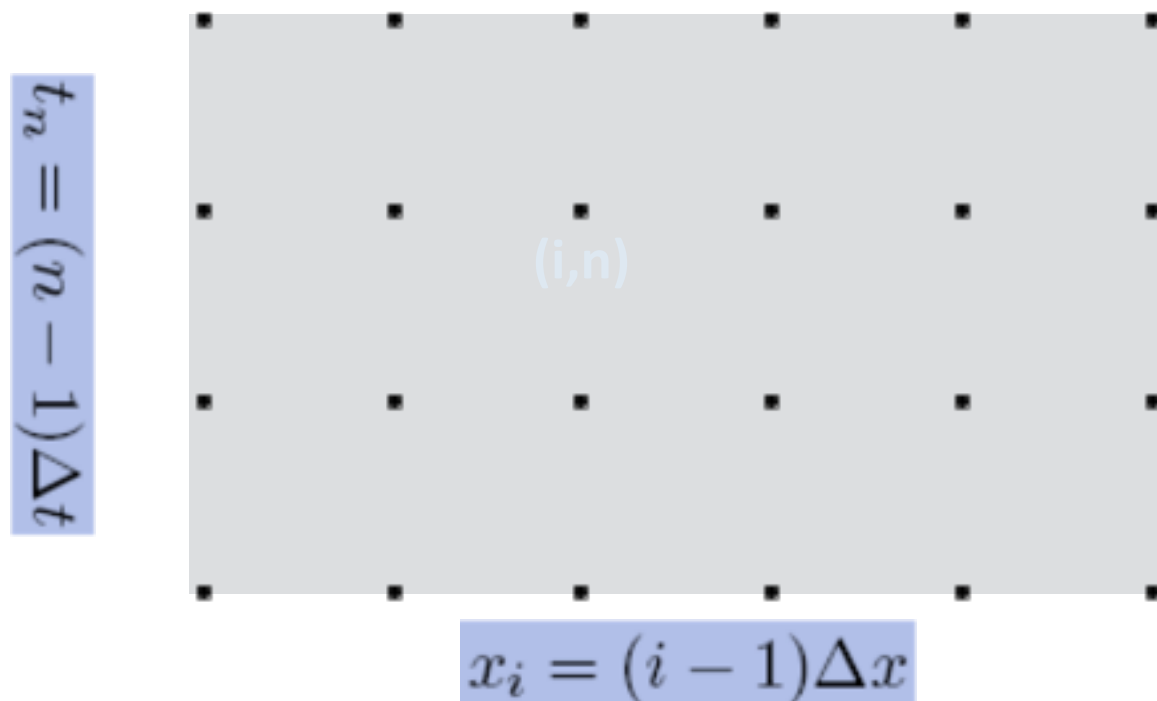
$$\rho(x_i)\partial_t v(x_i, t_n) = \partial_x T(x_i, t_n)$$

$$\partial_t T(x_i, t_n) = \kappa(x_i)\partial_x v(x_i, t_n)$$



# Pseudo-spectral method

## Derivatives



$$\tilde{F}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} dx$$
$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \tilde{F}(k) e^{ikx} dk$$

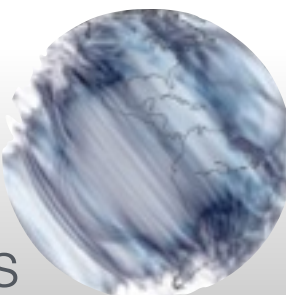
$$\int_{-\infty}^{+\infty} |f(x)| dx < \infty$$

temporal derivative: central differences

$$v_i^{n+1} = v_i^{n-1} + \frac{2\Delta t}{\rho_i} \times \left(\frac{\partial T}{\partial x}\right)_i^n$$
$$T_i^{n+1} = T_i^{n-1} + 2\Delta t \times \kappa_i \times \left(\frac{\partial v}{\partial x}\right)_i^n$$

spatial derivative: Fourier transforms

$$\frac{d}{dx} f(x) = \frac{d}{dx} \left[ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \tilde{F}(k) e^{ikx} dk \right]$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} ik \tilde{F}(k) e^{ikx} dk$$



# Pseudo-spectral method

## Recipe

$$\begin{aligned}\frac{d}{dx}f(x) &= \frac{d}{dx}\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\tilde{F}(k)e^{ikx}dk\right] \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}ik\tilde{F}(k)e^{ikx}dk\end{aligned}$$

- First, Fourier Transform whatever field  $f(x)$  we need to differentiate.
- Second, multiply each Fourier coefficient  $\tilde{F}(k)$  by  $ik$ .
- Finally, carry out inverse Fourier Transform to get desired derivatives.

