Pseudo-spectral methods

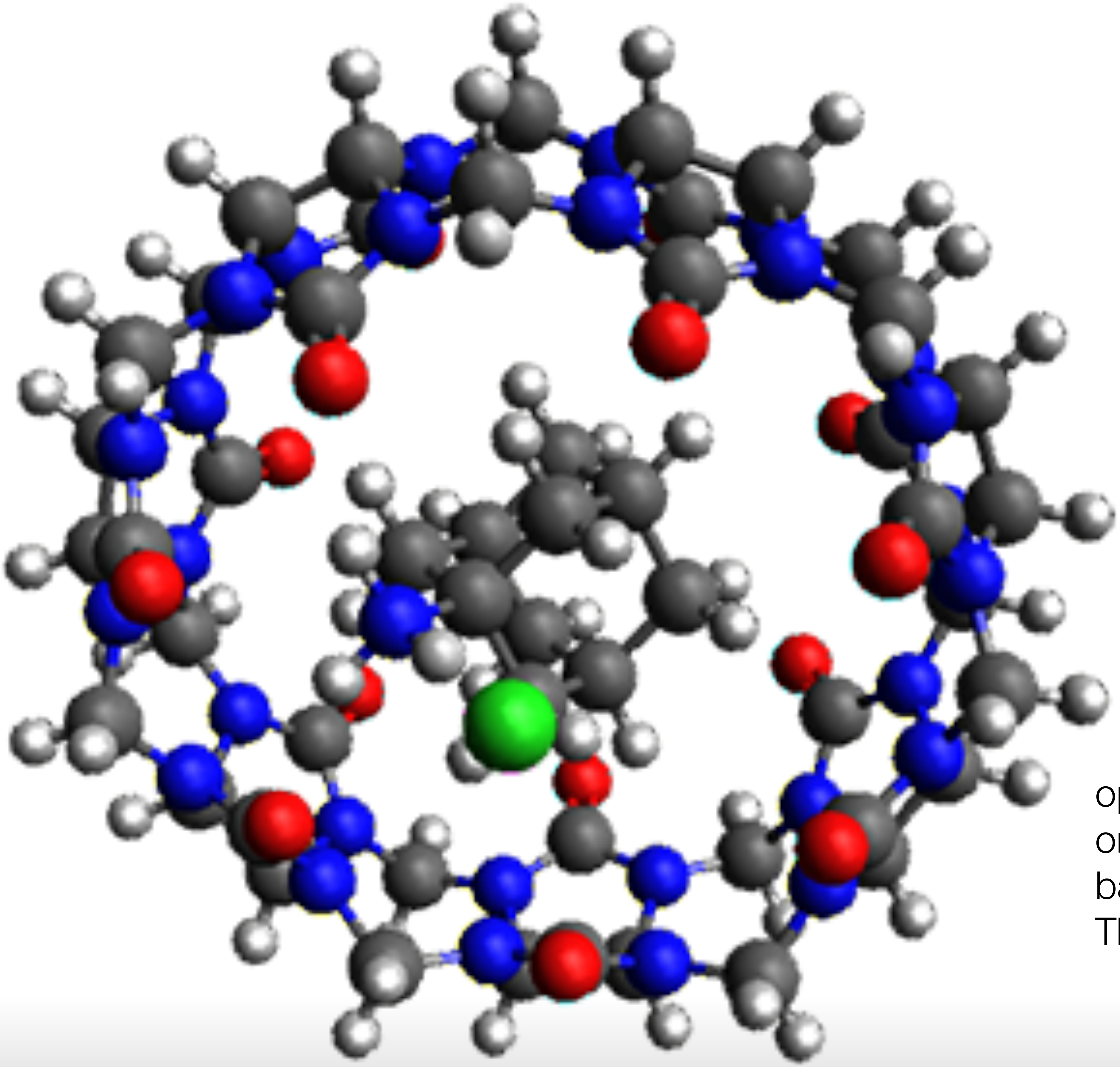
Galactic dynamics

Boltzmann equation

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

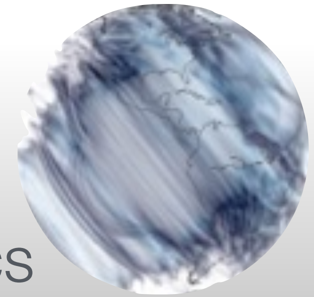
$\mathbf{F}$	Force field
f	probability density function
$\mathbf{p}$	momentum
m	particle mass

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
Ψ	wave function
V	potential energy
μ	“reduced” particle mass

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

Fluid dynamics

Navier-Stokes equation

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

P pressure field

$\mathbf{u}$ flow velocity vector

ν viscosity

ρ 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

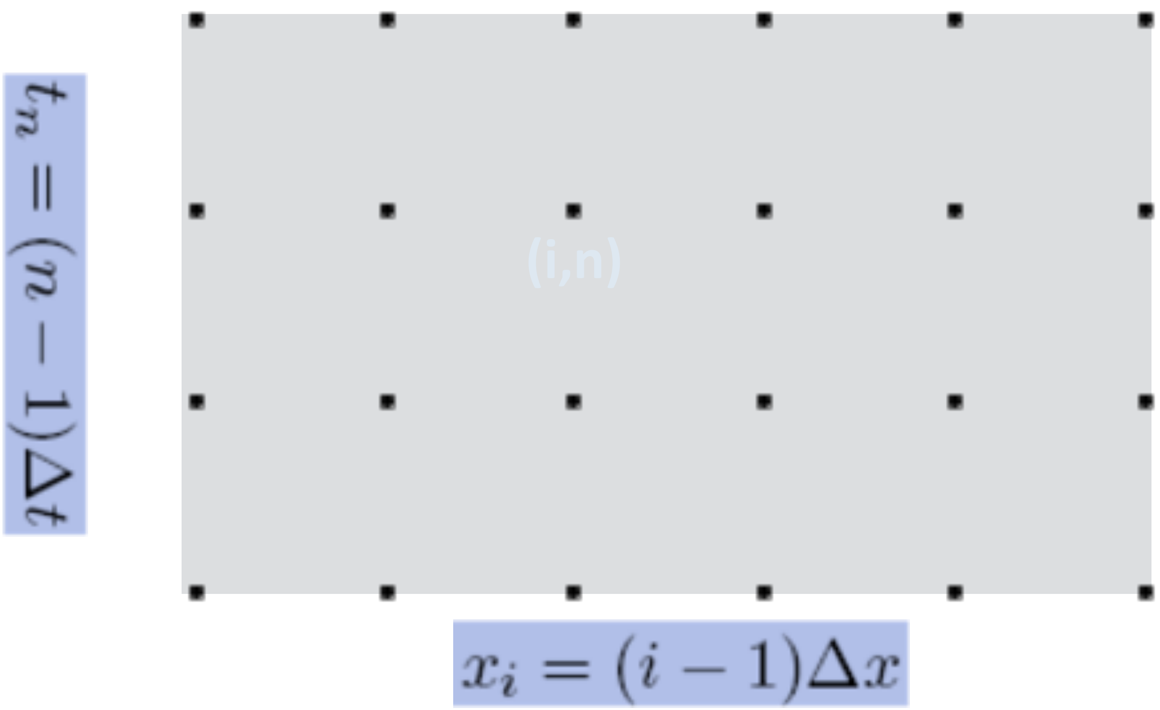
1st-order partial differential equations

$$\begin{aligned} \rho(x)\partial_t v(x,t) &= \partial_x T(x,t) \\ \partial_t T(x,t) &= \kappa(x)\partial_x v(x,t) \end{aligned}$$

$$\begin{aligned} v(x,t) &= \partial_t u(x,t) \\ T(x,t) &= \kappa(x)\partial_x u(x,t) \end{aligned}$$

Pseudo-spectral method

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



continuous form:

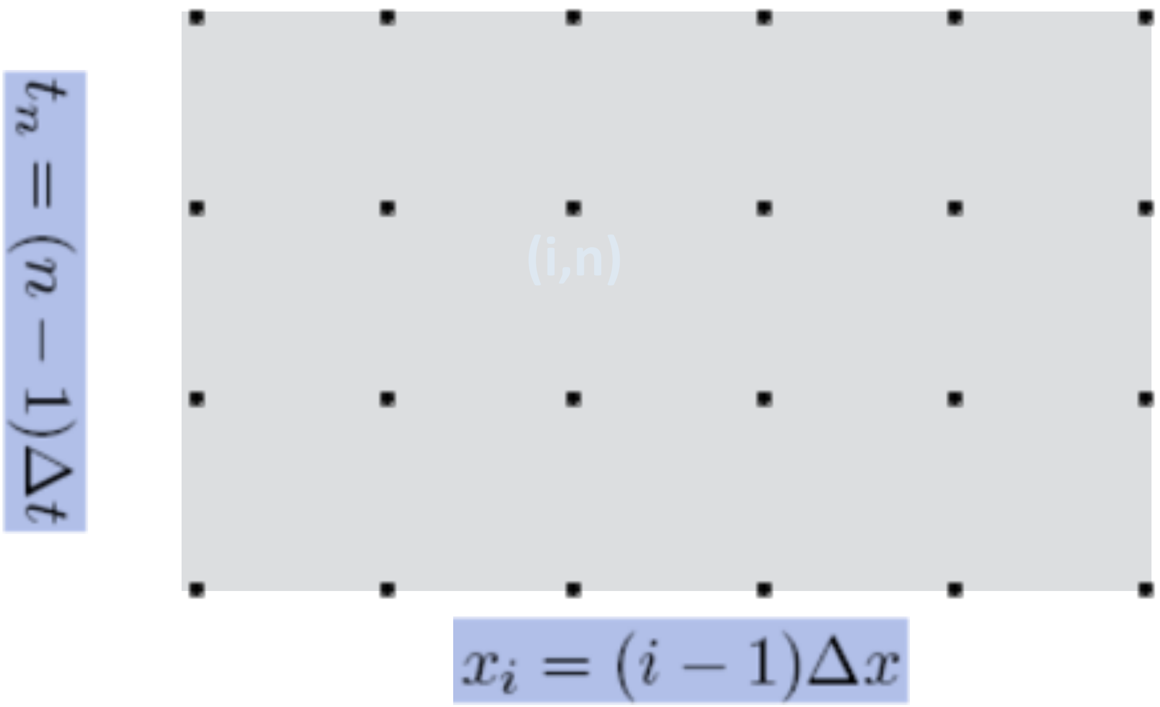
$$
\begin{aligned}
\rho(x)\partial_t v(x,t) &= \partial_x T(x,t) \\
\partial_t T(x,t) &= \kappa(x)\partial_x v(x,t)
\end{aligned}
$$

discretized form:

$$
\boxed{
\begin{aligned}
&\rho(x_i)\partial_t v(x_i,t_n) = \partial_x T(x_i,t_n) \\
&\partial_t T(x_i,t_n) = \kappa(x_i)\partial_x v(x_i,t_n)
\end{aligned}
}
$$

Pseudo-spectral method

Derivatives



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

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

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

temporal derivative: central differences

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

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

spatial derivative: Fourier transforms

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

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} ik\tilde{F}(k) e^{ikx} \mathrm{d}k$$

Pseudo-spectral method

Recipe

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

- 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.