Introduction to numerical modelling

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Content

- What is a model?
- Construction of a model
- Fickian diffusion
- Taylor series
- Stability
- Boundary conditions
- Numerical grids
- Types of ecosystem models

What is a model?

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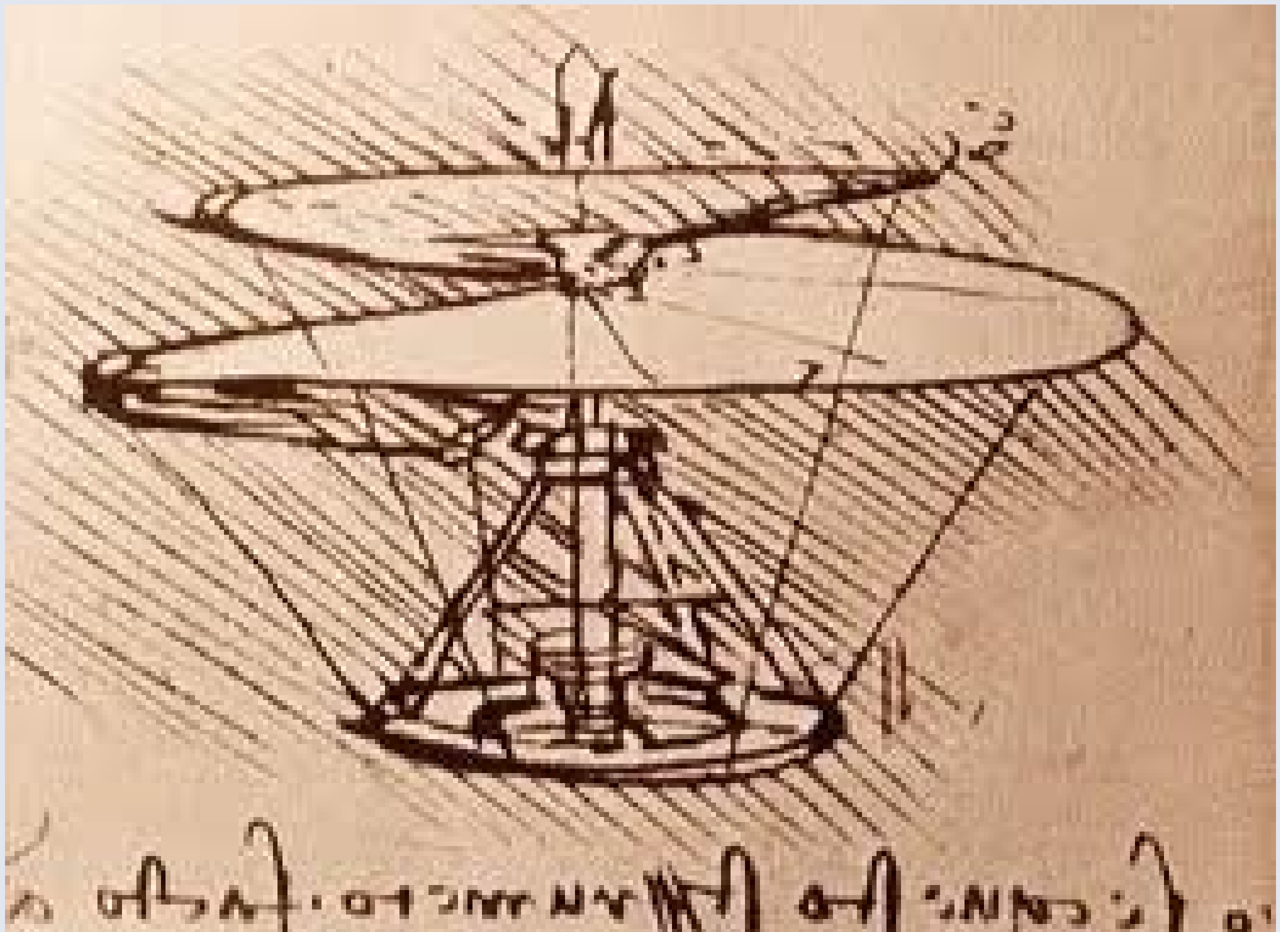


What is a model?

What is a model?

- In science, the word „MODEL“ has other, different meanings

- A model is a limited projection of reality
  - Projection (natural or artificial original)
  - Limitation (only relevant attributes)
  - Pragmatism (What? why? Etc.)
  - Validity

Stachowiak 1973

What is a model?

- Different meanings in different disciplines
  - Theory of science
  - Mathematics and logic
  - Mathematical models
  - Social sciences
  - Psychology
  - Educational science
  - Informatics

What is a model?

- Theory of science
  - In the methodology of theory of science models are used to explain known facts (objects) or they use hypothetical assumptions to test theories.
  - Explaining models (Scale models) have a relation to reality (toy car)
  - Analogy models create similarity in structure of reality e.g. planets and atomic model

What is a model?

- Social sciences
  - In research of social sciences an „Ideal typus“ (Max Weber) is an abstract, idealized model of reality; e.g. social structures (democracy or a medivial city) or temporal development (revolution or models of economic cycles)

What is a model?

- Mathematical models in science
  - Mathematical models are models expressed in equations based on e.g. physical laws
  - A validated model can be used for forecast (e.g. weather forecast)

Federal Ministry of Education and Research

Construction of a Model

- **Definition of an area**
- **Specific research project (goal?)**
- **Collection of information**
  - What is known from literature?
  - What is easy to measure?
- **First idealization**
  - What is important?
  - What can be neglected?
- **Second idealization**
  - Model formulation in the language of users
- **Third idealization**
  - formulation of the mathematical model
- **Fourth idealization**
  - Simplification of the mathematical model
- **Solution of the mathematical model**
- **Sensitivity analysis**
- **Interpretation of mathematical results**
  - Comparison with experimental data
  - Comparison with desired goal

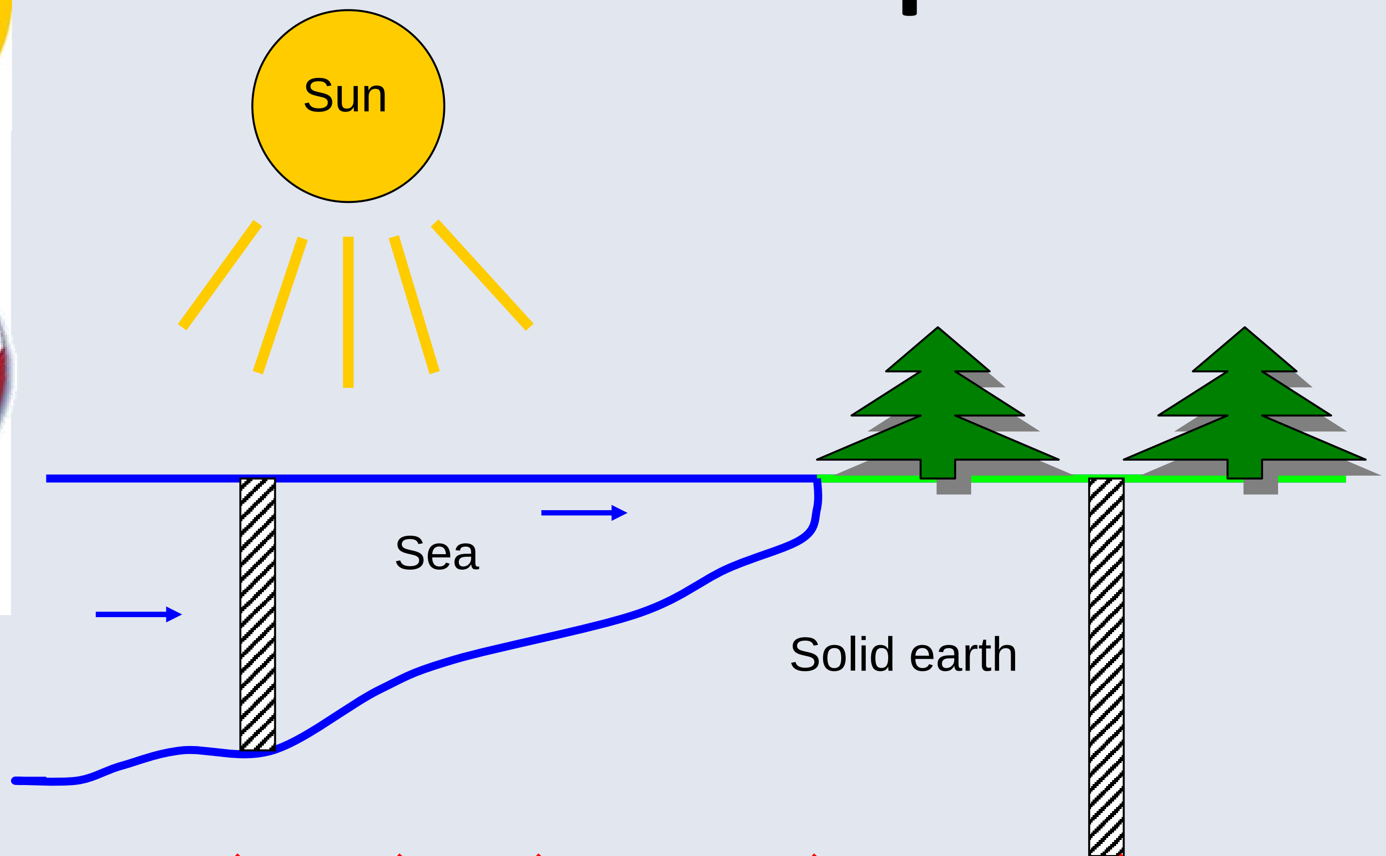
Types of Problems

- **Description of a situation**
  - Boundary value problem
- **Prediction**
  - initial condition problem
  - Given initial condition:
    - Definite solution -> deterministic
    - Indefinite solution -> bifurcation
    - Stochastic solution -> chaos
- **What was?**
  - Inverse problem
    - e.g. diffusion equation backward (not well posed)
- **Characteristic structures**
  - Eigen value problem
- **Identification problems**
  - Parameter estimation
  - Inverse problems (not well posed)

Basic Equations

- In the classical mechanics conservation equations exist for
  - Mass
  - Momentum
  - Energy
- In meteorology and oceanography for
  - Potential vorticity
  - Enstrophy
- In general, these equations are non-linear
- They cannot be solved analytically and must be solved numerically (Computer)
- Only special cases can be solved analytically (paper and pencil)

Example



$$\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}+w\frac{\partial T}{\partial z}=\frac{\partial}{\partial x}\left(D_l\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_l\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_v\frac{\partial T}{\partial z}\right)$$

Advection Diffusion

Classical Fickian Diffusion Equation

$$\frac{\partial T}{\partial t} = D_v \frac{\partial^2 T}{\partial z^2}$$

Taylor Series Expansion 1

$$f(x \pm \Delta x) = f(x) \pm \frac{\Delta x}{1!} f'(x) + \frac{\Delta x^2}{2!} f''(x) \pm \ldots + \frac{\Delta x^n}{n!} f^{(n)}(x)$$

$$f'(t) = \frac{\partial T}{\partial t} \qquad f''(t) = \frac{\partial^2 T}{\partial t^2}$$

$$T(t + \Delta t) = T(t) + \Delta t \frac{\partial T}{\partial t} + \frac{\Delta t}{2} \frac{\partial^2 T}{\partial t^2} + HOT$$

$$T(t - \Delta t) = T(t) - \Delta t \frac{\partial T}{\partial t} + \frac{\Delta t}{2} \frac{\partial^2 T}{\partial t^2} + HOT$$

Taylor Series Expansion 2

$$T(t+\Delta t) = T(t) + \Delta t \frac{\partial T}{\partial t} + \frac{\Delta t}{2} \frac{\partial^2 T}{\partial t^2} + HOT \qquad \mathbf{1}$$

$$T(t-\Delta t) = T(t) - \Delta t \frac{\partial T}{\partial t} + \frac{\Delta t}{2} \frac{\partial^2 T}{\partial t^2} + HOT \qquad \mathbf{2}$$

- 1: Forward difference $\frac{\partial T}{\partial t} = \frac{T(t+\Delta t) - T(t)}{\Delta t}$
- 2: Backward difference $\frac{\partial T}{\partial t} = \frac{T(t) - T(t-\Delta t)}{\Delta t}$
- 1-2: Central difference $\frac{\partial T}{\partial t} = \frac{T(t+\Delta t) - T(t-\Delta t)}{2\Delta t}$
- 1+2: central difference 2nd order

$$\frac{\partial^2 T}{\partial t^2} = \frac{T(t+\Delta t) + T(t-\Delta t) - 2T(t)}{\Delta t^2}$$

Taylor Series Expansion 3

$$f(x \pm \Delta x) = f(x) \pm \frac{\Delta x}{1!} f'(x) + \frac{\Delta x^2}{2!} f''(x) \pm \dots + \frac{\Delta x^n}{n!} f^{(n)}(x)$$

$$\frac{\partial T}{\partial t} = D_v \frac{\partial^2 T}{\partial z^2}$$

$$\alpha = \frac{D_v \Delta t}{\Delta z^2}$$

$$T(z,t+\Delta t) = T(z,t) + \alpha\left[T(z+\Delta z,t) + T(z-\Delta z,t) - 2T(z,t)\right]$$

Transition from a differential equation to a finite difference equation !

Basic Numerical Rule

Stability +

Consistency =

Convergence

Stability 1

$$T(z,t+\Delta t)=T(z,t)+\alpha\left[T(z+\Delta z,t)+T(z-\Delta z,t)-2T(z,t)\right]$$

$$\alpha=\frac{D_v\Delta t}{\Delta z^2}$$

- **Question:** which α ensures a stable solution?
- **Assumption:** Fourier decomposition: $T(z,t)=T_0\exp\left[i\left(kz-\omega t\right)\right]$
- **Solution:**

$$T(t+\Delta t)=T(t)\left[1-2\alpha\left(1-\cos k\Delta z\right)\right]$$

- Or:

$$T(t+\Delta t)=T(t)G$$

Stability 2

$$T(t+\Delta t) = T(t)G$$

- Stability:

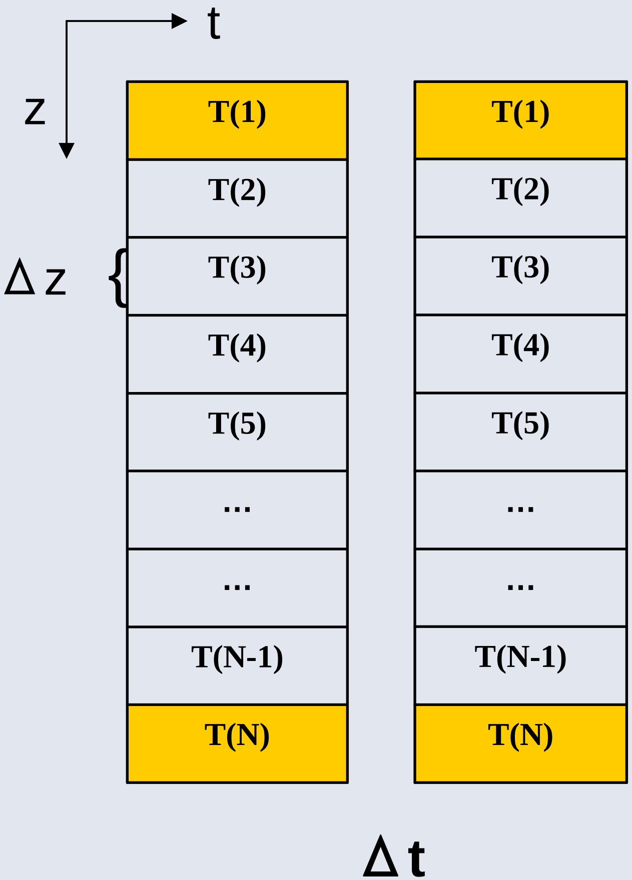
$$|G| \le 1$$

$$-1 \le 1 - 2\alpha(1 - \cos k\Delta z) \le 1$$

- RHS: stable for all $k \Delta z$
- LHS: critical value $(1 - \cos k\Delta z) = 2 \quad \mapsto \quad \alpha \le \frac{1}{2}$
- Stable solution: $\Delta t \le \frac{1}{2} \frac{\Delta z^2}{D_v}$

Organisation in the Computer

$$T(z,t+\Delta t) = T(z,t) + \alpha\left[T(z+\Delta z,t) + T(z-\Delta z,t) - 2T(z,t)\right]$$

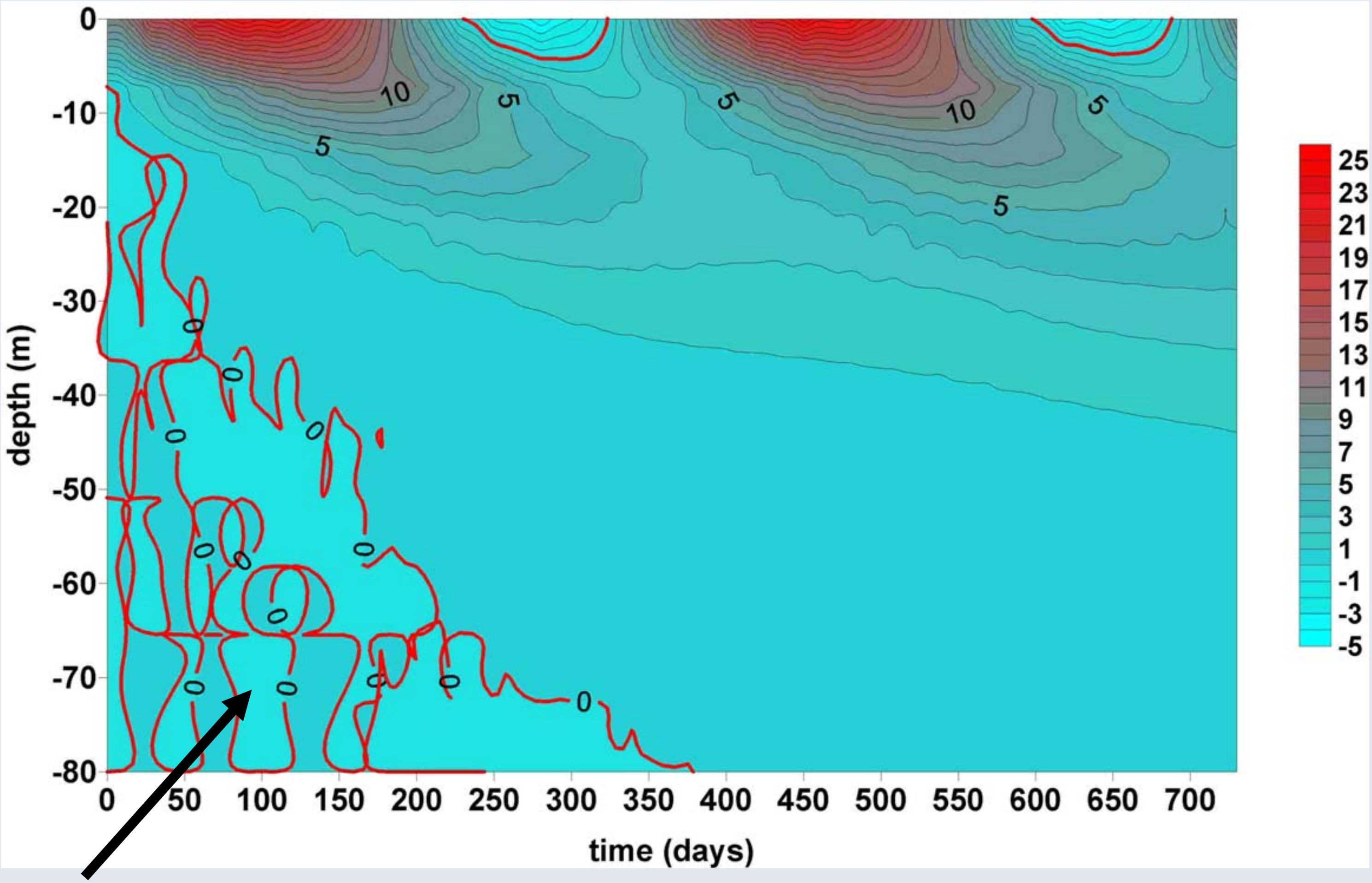


Boundary Conditions

$$T(t) = T_0 + T_1 \sin \sigma t_{\langle z=0 \rangle}$$

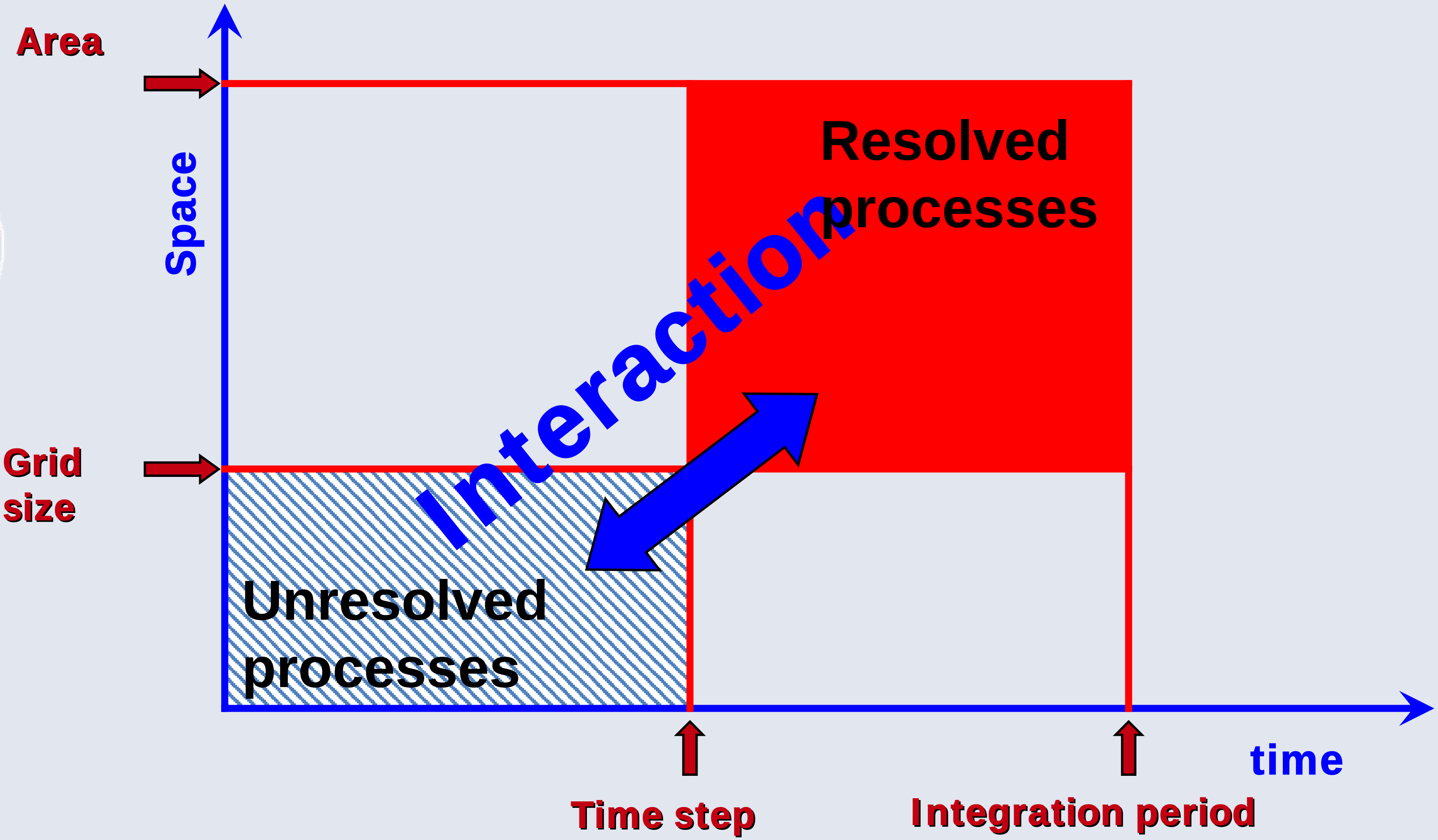
$$\frac{\partial T}{\partial z} = 0_{\langle z=\infty \rangle}$$

Solution

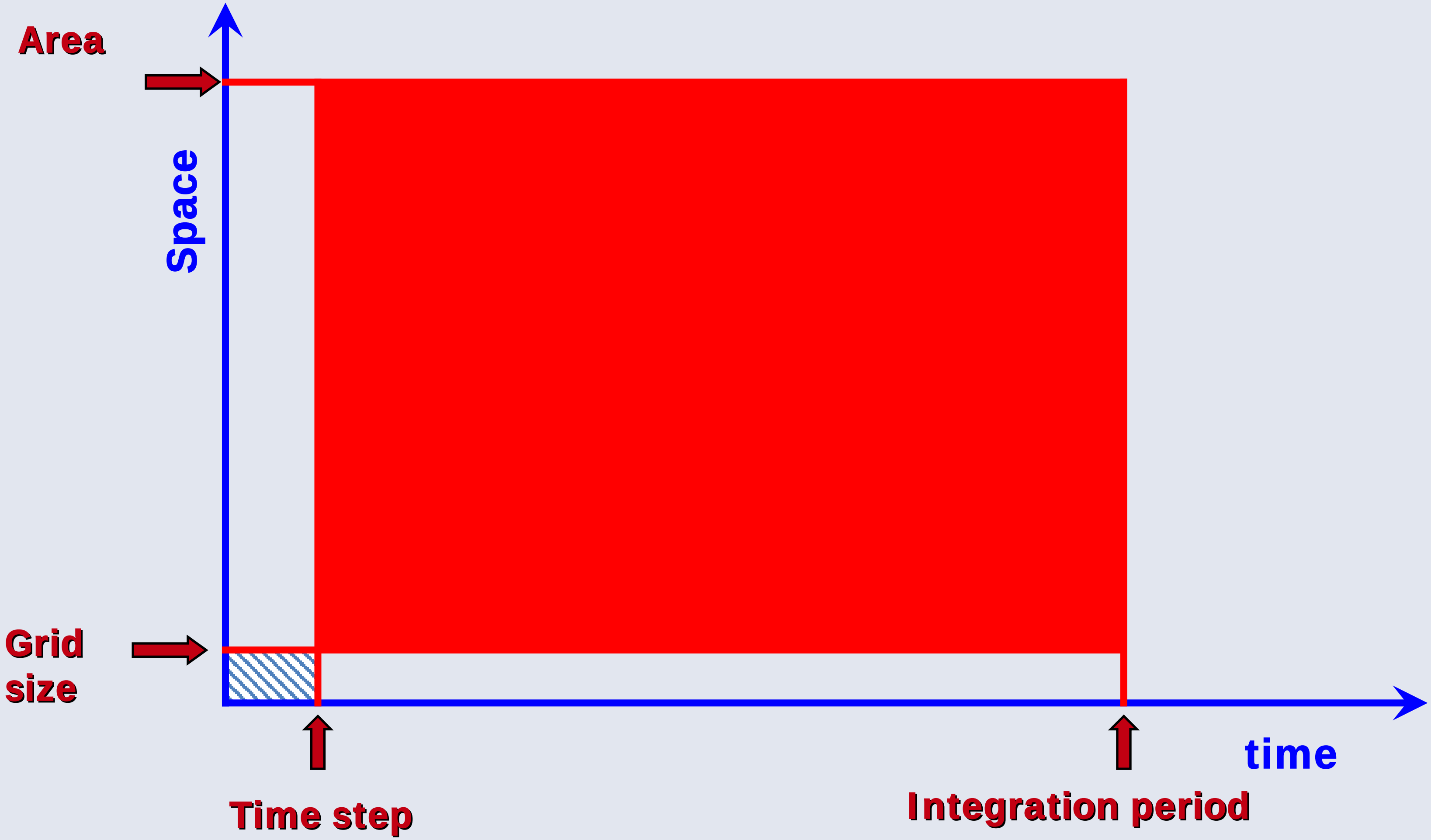


Model spin-up

Processes in 2 Dimensions



Processes in 2 Dimensions



Example from Oceanography 1

- Consider a one-dimensional channel without rotation and without friction:

$$\frac{\partial U}{\partial t} - gH\frac{\partial \zeta}{\partial x} = \frac{1}{\rho_0}\tau^{(x)}$$

Conservation of momentum

$$\frac{\partial \zeta}{\partial t} + \frac{\partial U}{\partial x} = 0$$

Conservation of mass

U = vertically integrated velocity, ζ = water elevation, g= gravity

H = water depth + ζ, ρ_0 = reference density, $\tau^{(x)}$ = wind stress

$\partial / \partial t$ and $\partial / \partial x$ are partial derivatives in time an space

Example from Oceanography 2

The system

$$\frac{\partial U}{\partial t} - gH\frac{\partial \zeta}{\partial x} = \frac{1}{\rho_0}\tau^{(x)}$$

$$\frac{\partial \zeta}{\partial t} + \frac{\partial U}{\partial x} = 0$$

Can be written as

$$\begin{bmatrix} \frac{\partial}{\partial t} & -gH\frac{\partial}{\partial x} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial t} \end{bmatrix} * \begin{bmatrix} U \\ \zeta \end{bmatrix} = \begin{bmatrix} \frac{1}{\rho_0}\tau^{(x)} \\ 0 \end{bmatrix}$$

Or: **A * X = F** with A = system dynamics matrix,
X = desired solution
F = forcing

Example from Oceanography 3

- The dynamics of the system is in the matrix

$$\begin{bmatrix} \frac{\partial}{\partial t} & -gH\frac{\partial}{\partial x} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial t} \end{bmatrix}$$

- Using a Fourier approach:

$$U,\zeta \quad \approx \quad e^{i(kx-\sigma t)}$$

$$\begin{bmatrix} -i\sigma & -ikgH \\ ik & -i\sigma \end{bmatrix} \quad with \quad \sigma = \frac{2\pi}{T} \quad and \quad k = \frac{2\pi}{L}$$

Example from Oceanography 4

$$\det\begin{bmatrix} -i\sigma & -ikgH \\ ik & -i\sigma \end{bmatrix} = 0$$

$$-\sigma^2 + gHk^2 = 0 \quad \Rightarrow \quad \frac{\sigma^2}{k^2} = c^2 = gH$$

$$c = \sqrt{gH}$$

Fundamental property in geophysical fluid dynamics

Shallow water equations (SWE)

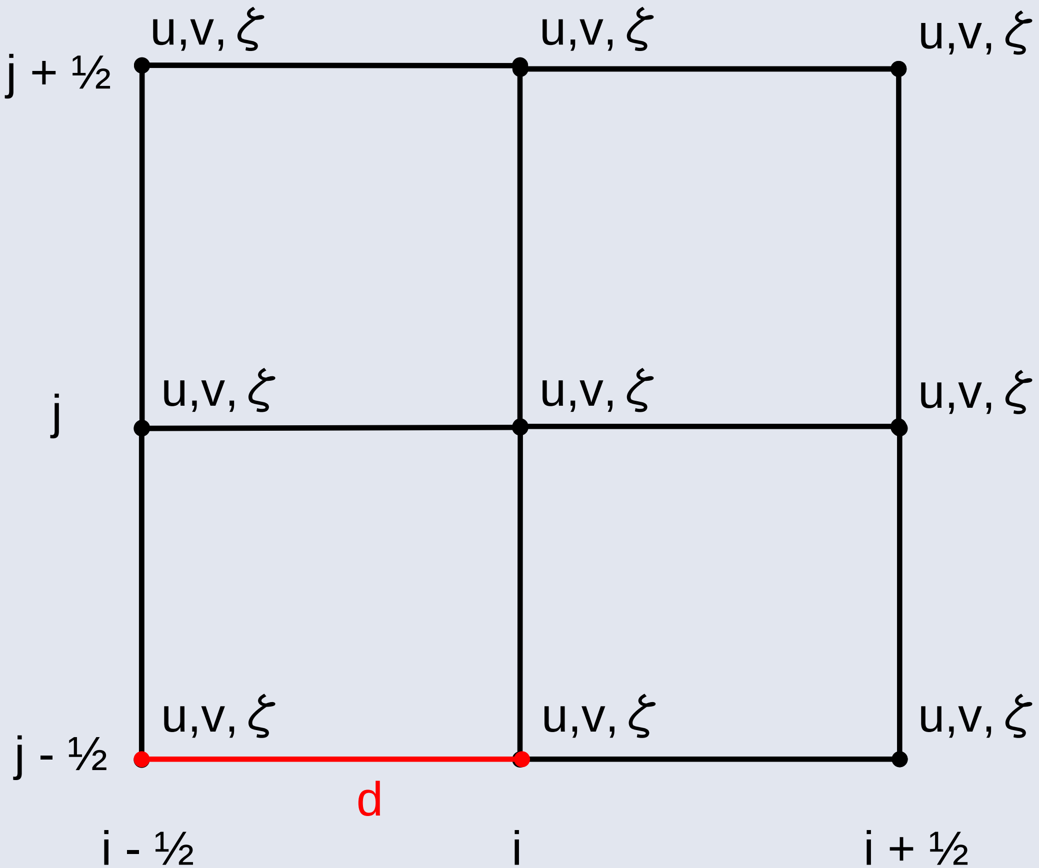
$$\frac{\partial u}{\partial t} - fv + g\frac{\partial \zeta}{\partial x} = 0$$

$$\frac{\partial v}{\partial t} + fu + g\frac{\partial \zeta}{\partial y} = 0$$

$$\frac{\partial \zeta}{\partial t} + H\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) = 0$$

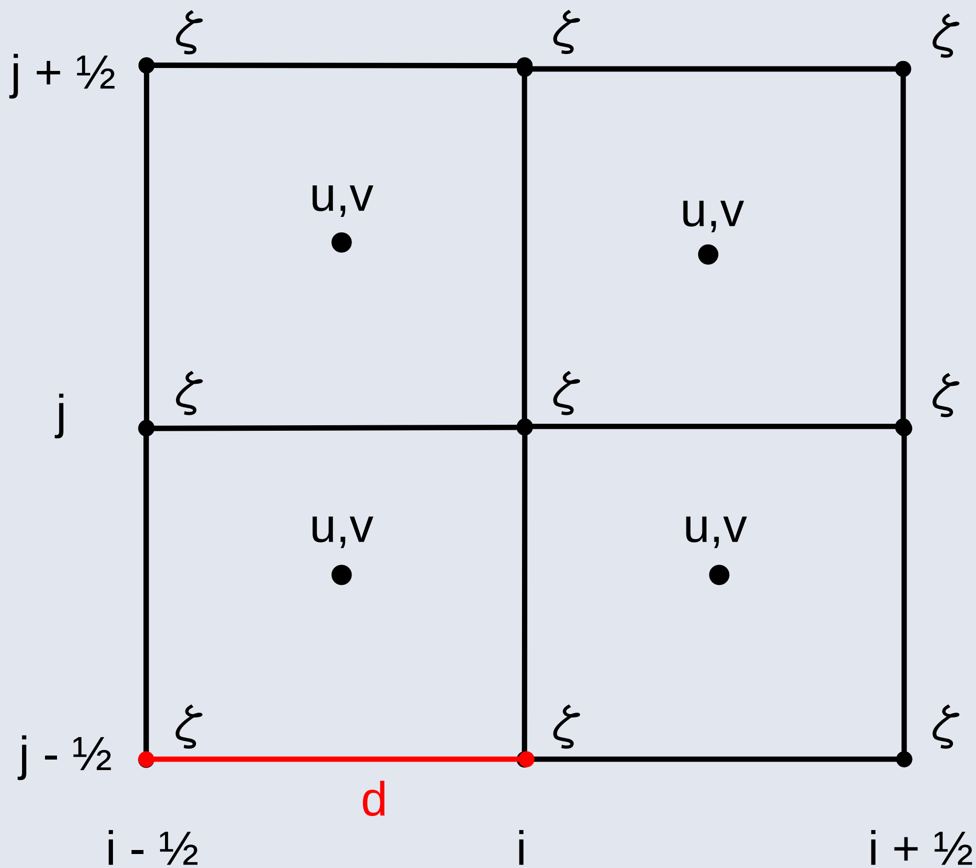
Question: How to organize the grid?

A-grid



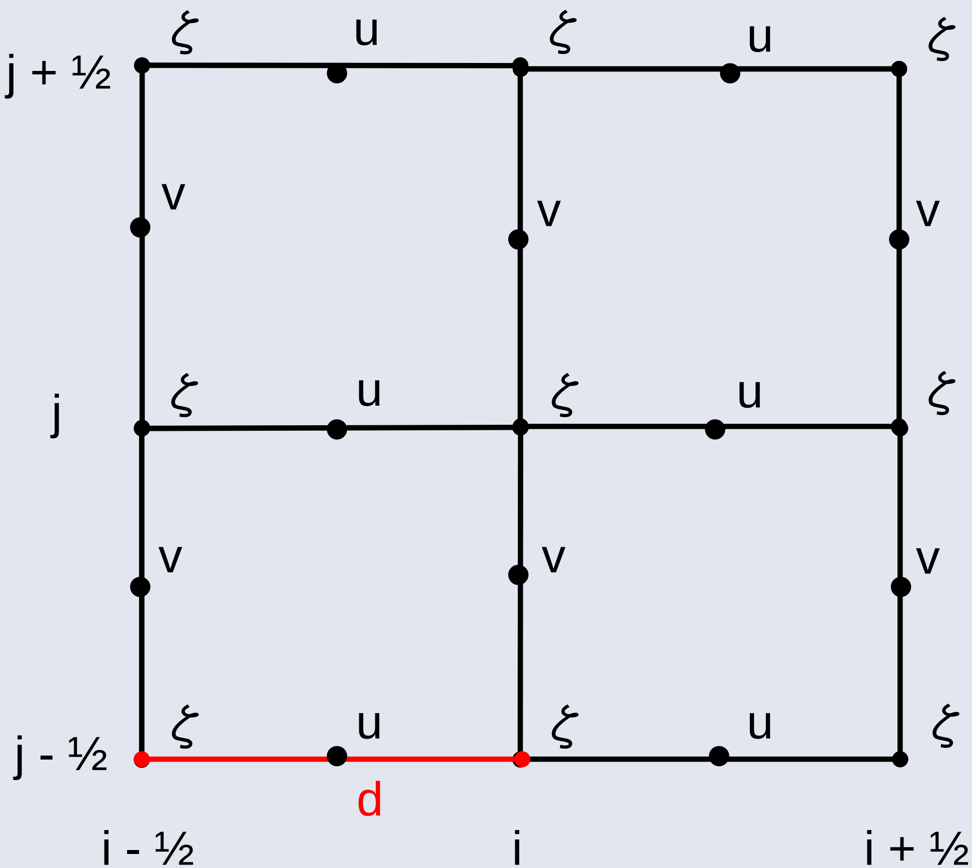
Arakawa & Lamb 1977

B-grid



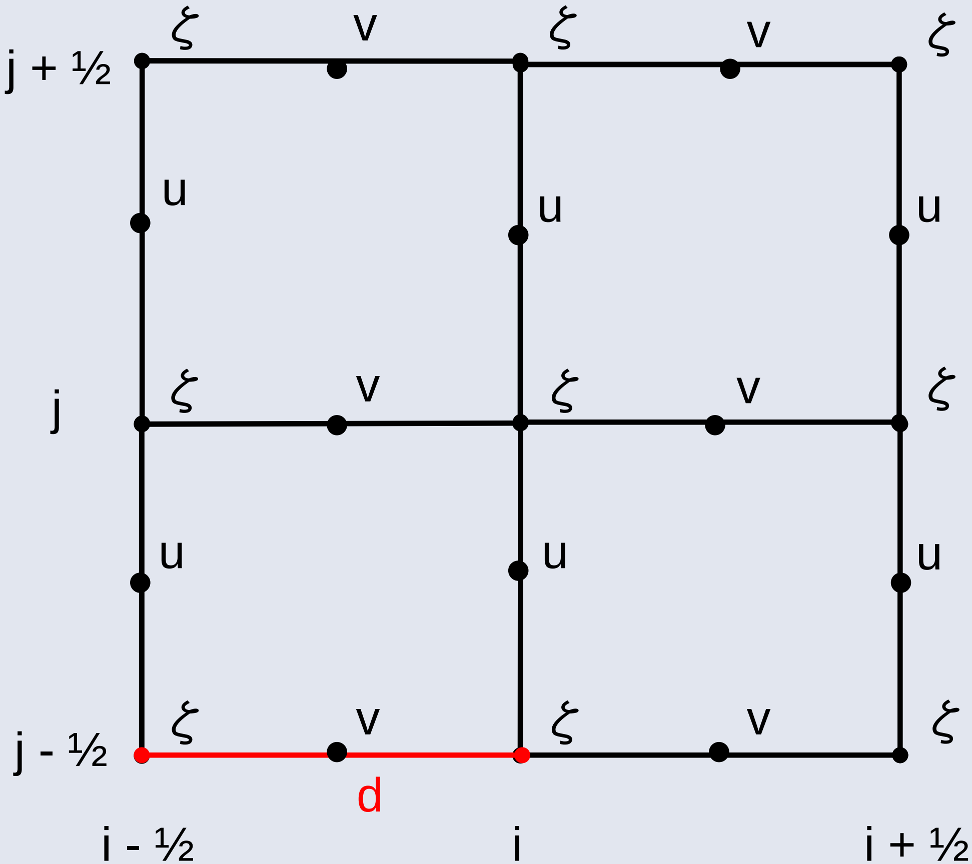
Arakawa & Lamb 1977

C-grid



Arakawa & Lamb 1977

D-grid



Arakawa & Lamb 1977

SWE in A-grid

$$\frac{\partial u}{\partial t} - fv + (g/d)\left(\overline{\delta_x \zeta}^x\right) = 0$$

$$\frac{\partial v}{\partial t} + fu + (g/d)\left(\overline{\delta_y \zeta}^y\right) = 0$$

$$\frac{\partial \zeta}{\partial t} + (H/d)\left(\overline{\delta_x u}^x + \overline{\delta_y v}^y\right) = 0$$

$$(\delta_x \alpha)_{i,j} \equiv \alpha_{i+1/2,j} - \alpha_{i-1/2,j}$$

$$(\overline{\alpha}^x)_{i,j} \equiv \tfrac{1}{2}(\alpha_{i+1/2,j} + \alpha_{i-1/2,j})$$

Arakawa & Lamb 1977

SWE in C-grid

$$\frac{\partial u}{\partial t} - f\overline{v}^{xy} + (g/d)(\delta_x \zeta) = 0$$

$$\frac{\partial v}{\partial t} + f\overline{u}^{xy} + (g/d)(\delta_y \zeta) = 0$$

$$\frac{\partial \zeta}{\partial t} + (H/d)\left(\delta_x u + \delta_y v\right) = 0$$

$$(\delta_x \alpha)_{i,j} \equiv \alpha_{i+1/2,j} - \alpha_{i-1/2,j}$$

$$(\overline{\alpha}^x)_{i,j} \equiv \tfrac{1}{2}(\alpha_{i+1/2,j} + \alpha_{i-1/2,j})$$

Arakawa & Lamb 1977

How good are these grids?

$$\frac{\partial u}{\partial t} - fv + g\frac{\partial \zeta}{\partial x} = 0$$

$$\frac{\partial v}{\partial t} + fu = 0$$

$$\frac{\partial \zeta}{\partial t} + H\frac{\partial u}{\partial x} = 0$$

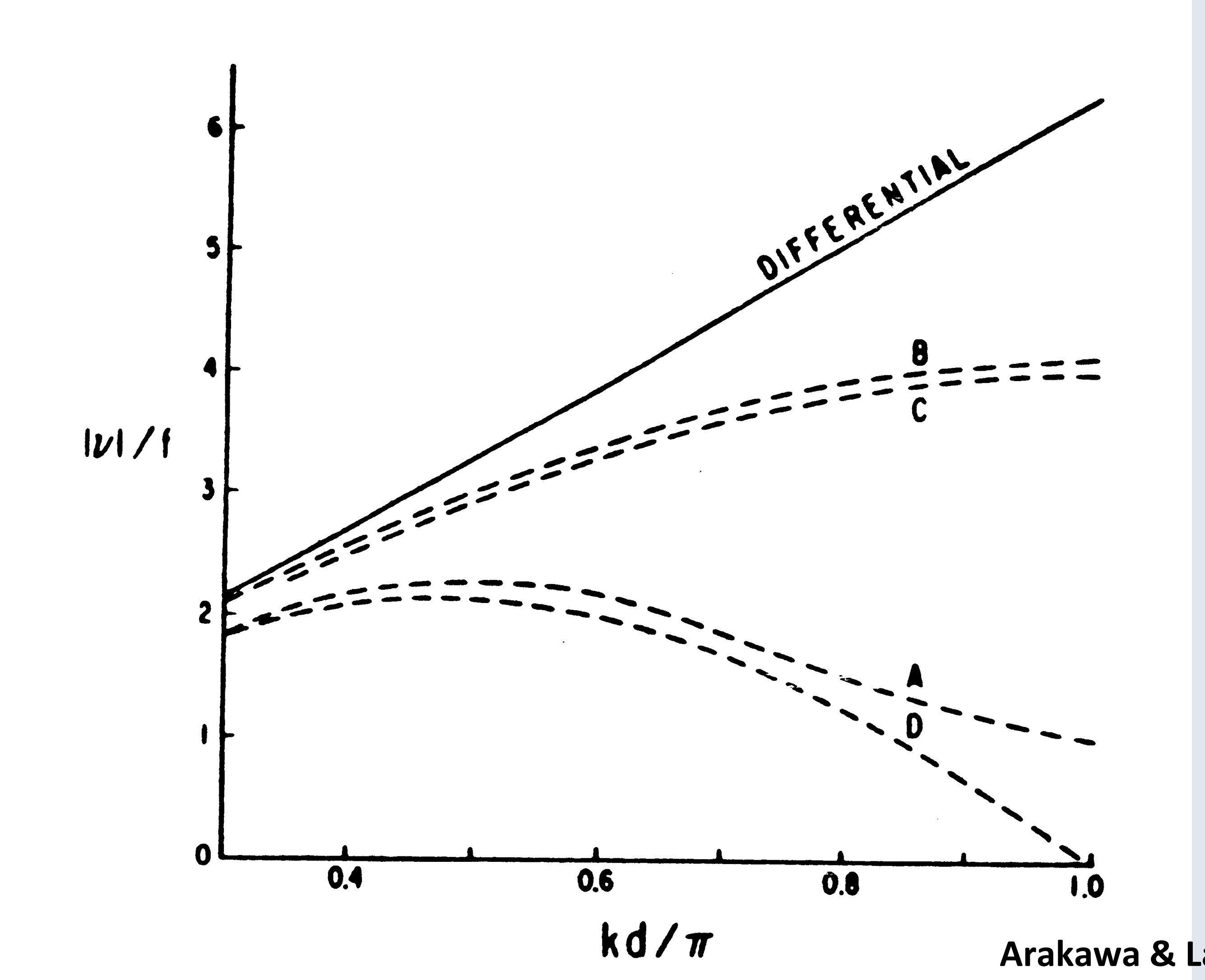
$$\frac{\partial^2 u}{\partial t^2} + f^2 u - gH\frac{\partial^2 u}{\partial x^2} = 0$$

$$u \sim \exp[i(kx - \omega t)]$$

$$(\omega / f)^2 = 1 + gH(k/f)^2$$

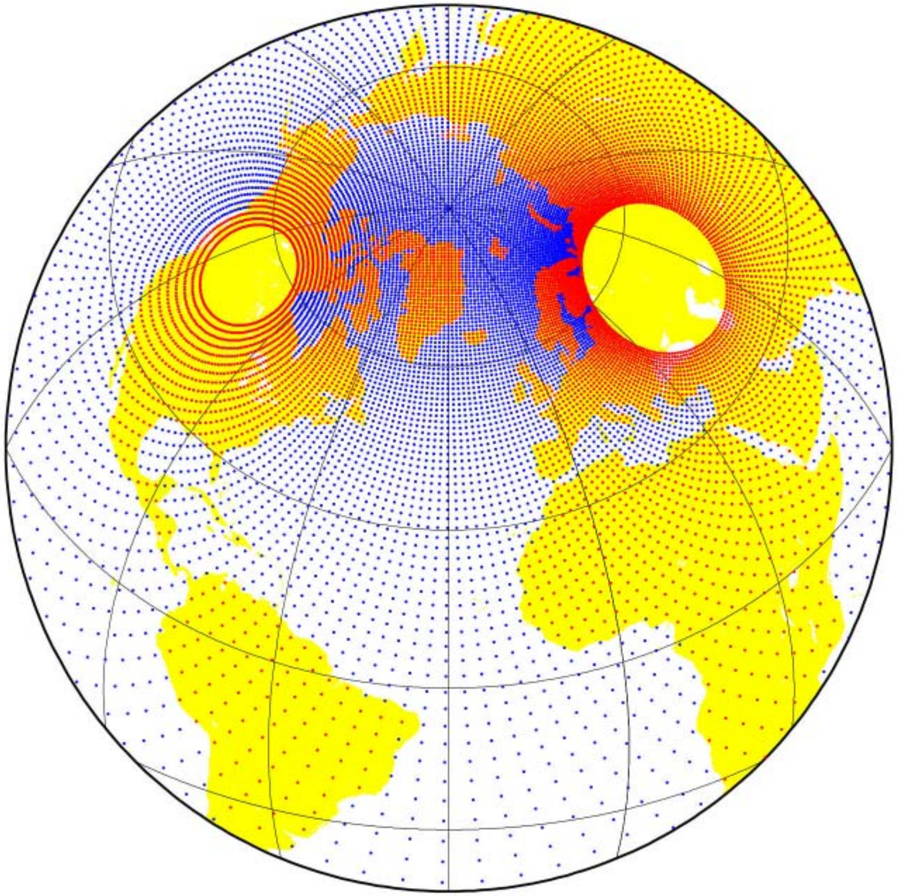
Arakawa & Lamb 1977

Solutions



Arakawa & Lamb 1977

Bi-polar grid



Marsland et al. 2003

ADR - Equation

- A = advection
- D = diffusion
- R = reaction

$$\frac{\partial q}{\partial t} + v_j \frac{\partial q}{\partial x_j} = \frac{\partial}{\partial x_j}\left(D_j \frac{\partial q}{\partial x_j} \right) + S$$

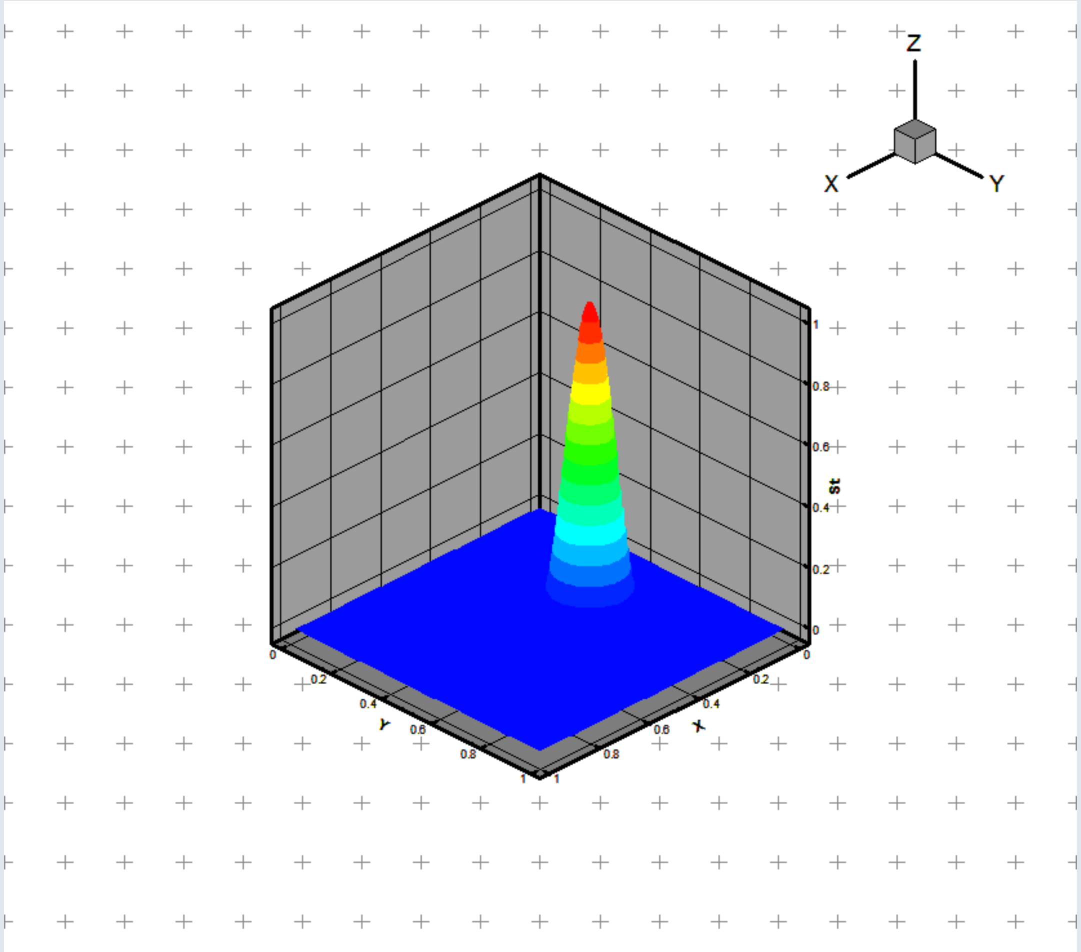
$q = q(x_i, t)$ $v_j = v_j(x_i, t)$ $D_j = D_j(x_i, t)$ $S = S(x_i, t)$

ADR - Equation

- Advection only

$$\frac{\partial q}{\partial t} + v_j \frac{\partial q}{\partial x_j} = \frac{\partial}{\partial x_j}\left(D_j \frac{\partial q}{\partial x_j} \right) + S$$

Example: Advection



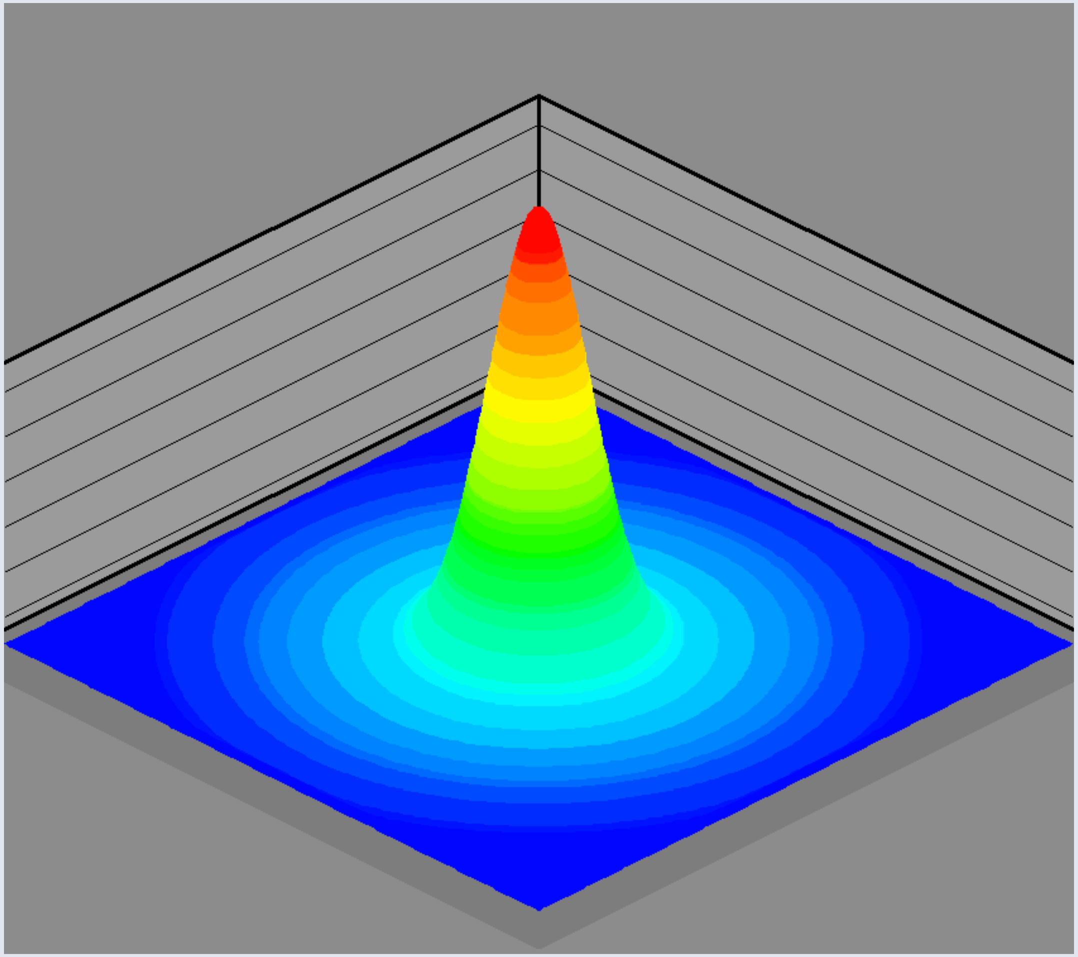
With kind permission of Mohammadi-Aragh

ADR - Equation

- Diffusion only

$$\frac{\partial q}{\partial t} + \cancel{v_j \frac{\partial q}{\partial x_j}} = \frac{\partial}{\partial x_j}\left(D_j \frac{\partial q}{\partial x_j} \right) + \cancel{S}$$

Example: Diffusion



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ADR - Equation

- Reaction only e.g.
  - Growth
  - Radioactive decay

$$\frac{\partial q}{\partial t} + v_j \frac{\partial q}{\partial x_j} = \frac{\partial}{\partial x_j}\left(D_j \frac{\partial q}{\partial x_j} \right) + S$$

Ecosystem models

- Thermodynamical models
- Analysis tools
  - Growth models
  - Allometric models
  - Network analysis
- Compartment models

Thermodynamical models

- Analogy to classical thermodynamics
- Life is a dissipative structure far from equilibrium
  - Organism-environment relationship
    - Von Uexküll (1926)
  - Maximum power principle
    - Odum & Pinkerton (1955)
  - Non-equilibrium thermodynamics
    - Prigogine (1955)
- Try to understand evolution
  - Emergy (embodied energy)
  - Exergy
  - Ascendency

Analysis tools

- Growth models
  - 20-30 equations describing growth
  - Including Pütter-Bertalanffy, Zotina-Zotin, Robertson, Richards, Gomperts
  - Plant growth, mammals, birds, tumors, fishes, invertebrates etc.
- An irreducible unification results in 3 equations

$$\frac{1}{W}\frac{dW}{dt} = K_g\left(\frac{W_m^b}{W^b} - 1\right) \qquad \frac{1}{W}\frac{dW}{dt} = K_d(t_m - t) \qquad \frac{1}{W}\frac{dW}{dt} = K_f(W_m - W)$$

Analysis tools

- Allometric models
  - An ataxonomic ecosystem conception in terms of size or mass spectra
  - Allometry (similarity analysis or biological scaling)

$$y = aM^b$$

  - Advantage: fast computation
  - Disadvantage: size spectrum

Analysis models

- Network analysis
  - Dealing with better understanding of the internal dynamics of the system and the non-linear interaction for food chain or complex food webs

Compartment models

- food web model
- trophic level model
- trophic categories model
- functional group model
- generic model
- Individual based models (IBM)

- ADR equations

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Thanks for listening