Finite differences method

Introduction to Lithospheric Geodynamic Modelling

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Contents

- How to transform partial differential equations to something computers understand
- Finite differences method (FDM)
    - Application to the heat equation
    - Comparison with analytical results
    - Boundary and initial conditions in FDM
    - Stability and accuracy of solutions

Motivation

- Analytical solutions to heat diffusion and material flow
  - Give good insight into the processes in question
  - Are *exact* and *provable* to be correct
  - Need to be re-derived when boundary/initial conditions change or new terms are added
  - Do not exist at all in some (many) cases

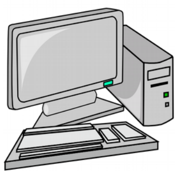
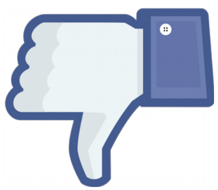
➔ Numerical methods
  - Computer algorithms to solve partial differential equations of many kind
  - Almost exactly opposite pros/cons

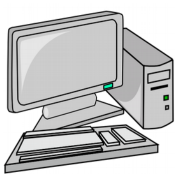
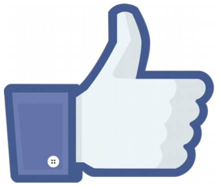
Finite differences method (FDM)

- Based on idea of approximating derivatives of functions with *finite differences* that can be evaluated with a computer
  - This approximation is done only at discrete locations (grid points) → accuracy
  - Relatively easy to implement
- Other methods used in geodynamics, e.g. finite element or finite volume methods (FEM, FVM)
  - Used to solve same PDEs but use different mathematical background
  - Concepts of discretization, initial conditions and boundary conditions apply

Finite differences method (FDM)

- What is FDM?
- Basic idea:

 & $\frac{\mathrm{d}f}{\mathrm{d}x}$ –> 

 & $\frac{1+5}{6-1}$ –> 

Finite differences method (FDM)

- How to apply FDM to the heat diffusion equation?
- Basic idea:

$$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=x_1} = \lim_{x_2 \to x_1} \frac{f(x_2) - f(x_1)}{x_2 - x_1} = \lim_{\Delta h \to 0} \frac{f(x_1 + \Delta h) - f(x_1)}{\Delta h}$$

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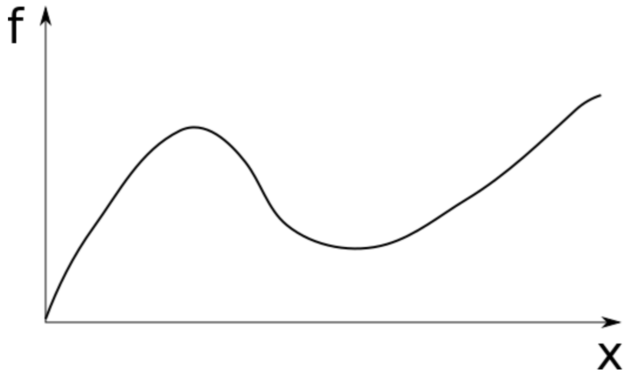
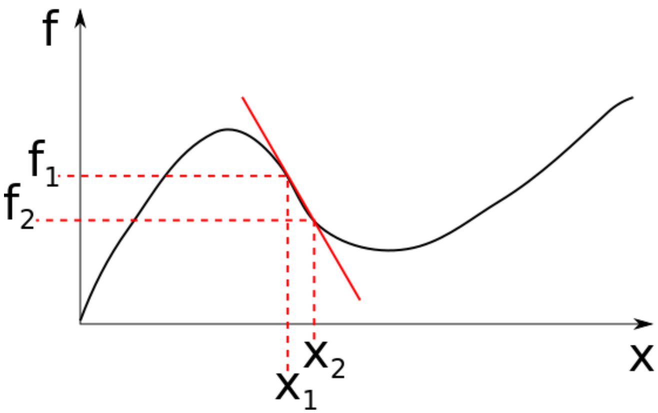
$$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=x_1} \approx \frac{f(x_2) - f(x_1)}{x_2 - x_1} = \frac{f(x_1 + \Delta h) - f(x_1)}{\Delta h}$$

… where $x_2 – x_1$ is small (or small enough)

Finite differences method (FDM)





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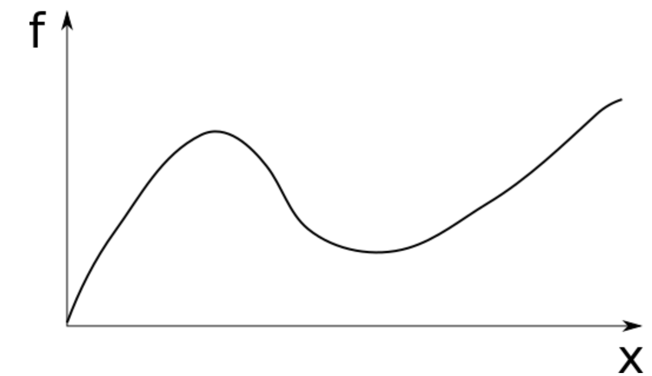
Finite differences method (FDM)



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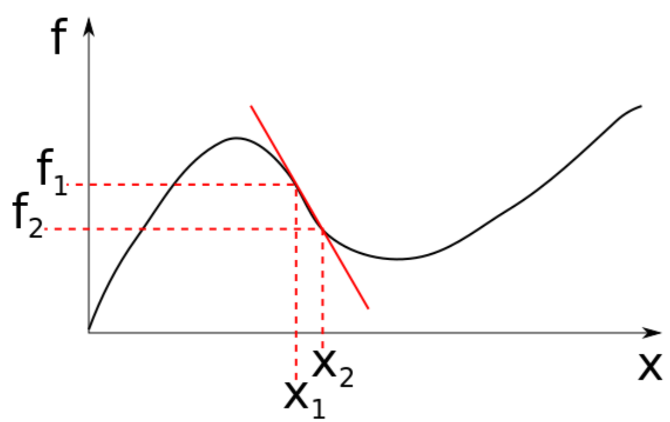
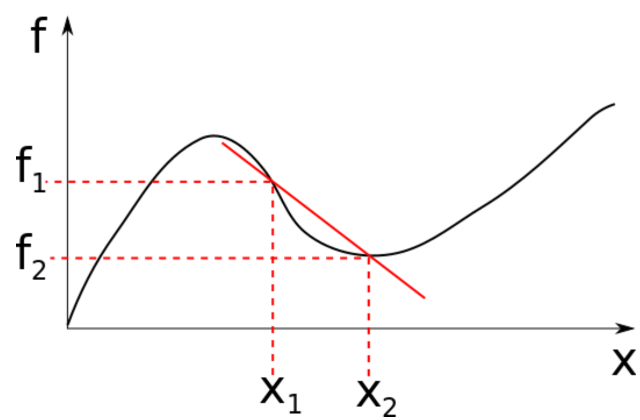
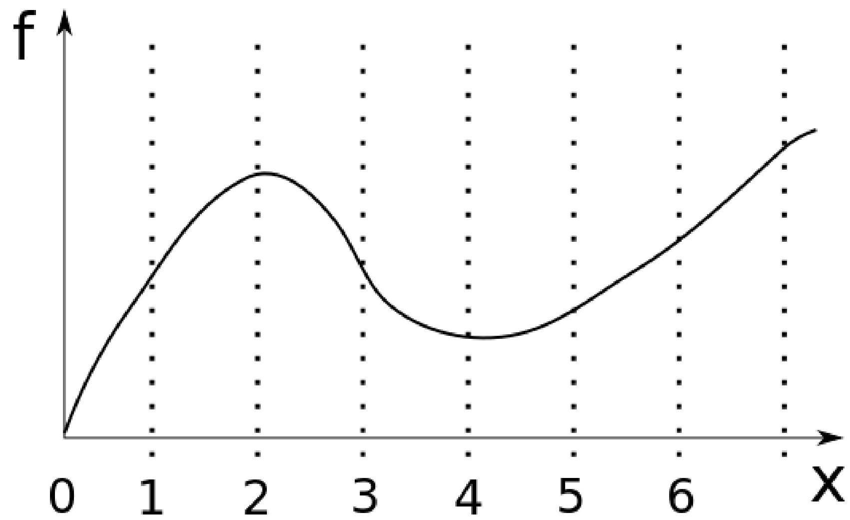




Grid

Grid number: 0, 1, 2, 3, …
Grid location: x_0, x_1, x_2, ...

$$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=x_1} = f'(x_1) \approx \frac{f_2 - f_1}{x_2 - x_1}$$



$$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=x_i} = f'(x_i) \approx \frac{f_{i+1} - f_i}{x_{i+1} - x_i}$$

Forward, backward and central differences

Forward:

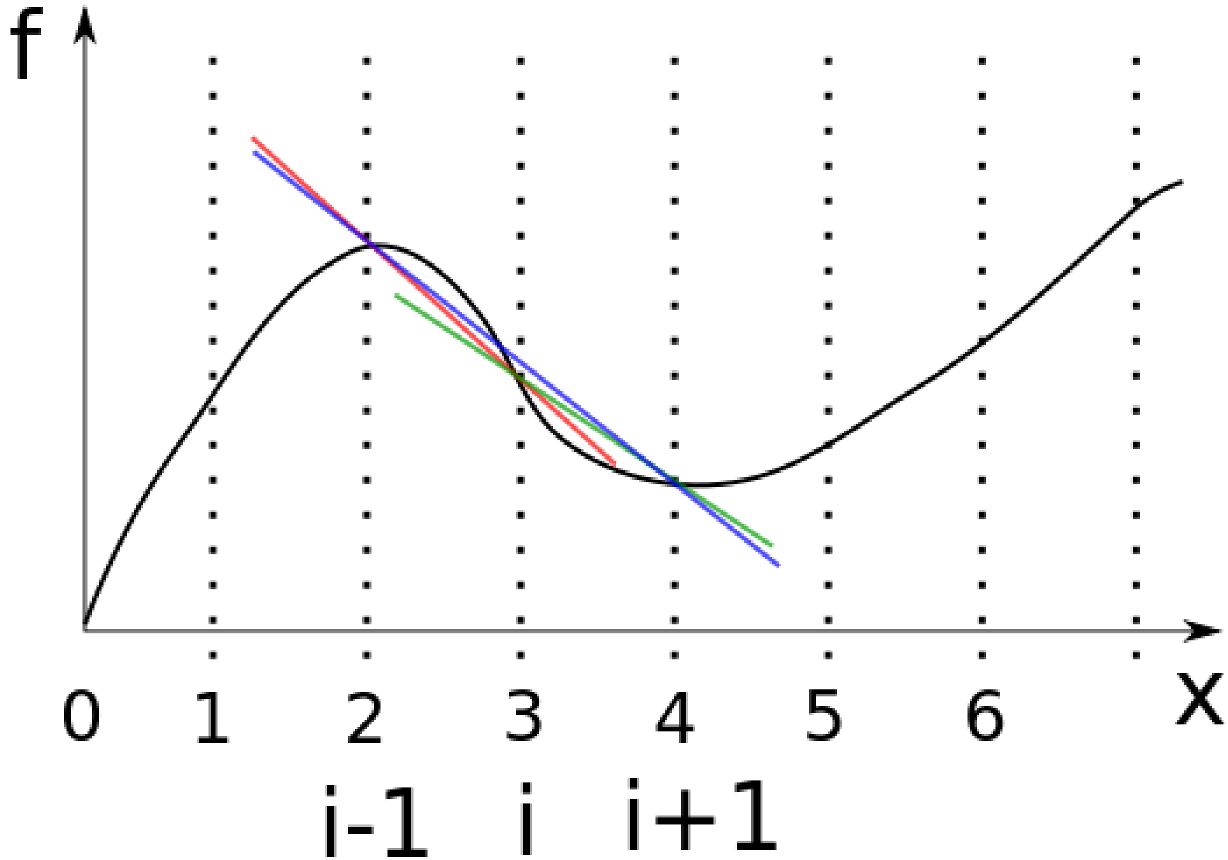
$$f'(x_i) \approx \frac{f_{i+1} - f_i}{x_{i+1} - x_i}$$

Backward:

$$f'(x_i) \approx \frac{f_i - f_{i-1}}{x_i - x_{i-1}}$$

Central:

$$f'(x_i) \approx \frac{f_{i+1} - f_{i-1}}{x_{i+1} - x_{i-1}}$$



Example 1: FDM for heat flow

$$q = k\frac{\mathrm{d}T}{\mathrm{d}z}$$

discretization

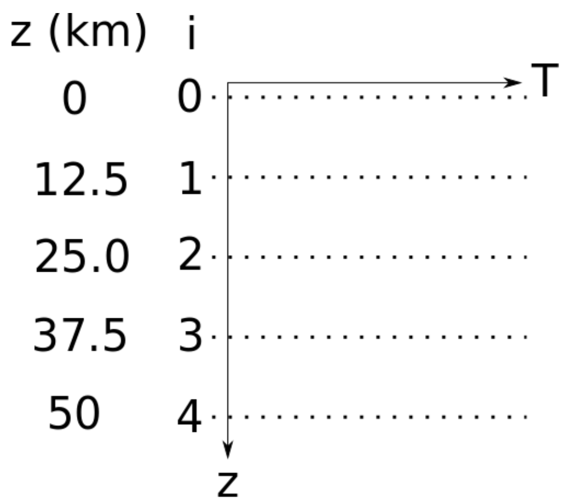
$$q = k\frac{T_i - T_{i-1}}{z_i - z_{i-1}}$$

rearrange

$$T_i = \frac{q}{k}(z_i - z_{i-1}) + T_{i-1}$$

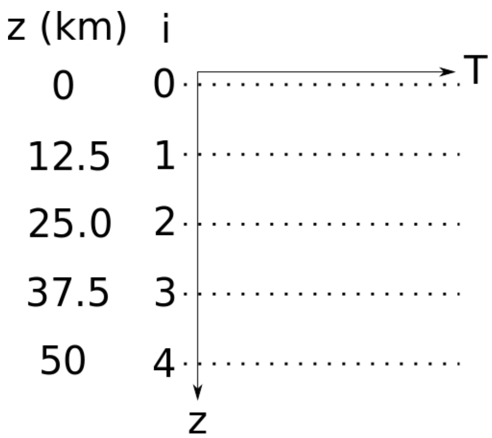
choose grid

- num of grid points
- boundary locations



Example 1: FDM for heat flow

$$T_i = \frac{q}{k}(z_i - z_{i-1}) + T_{i-1}$$



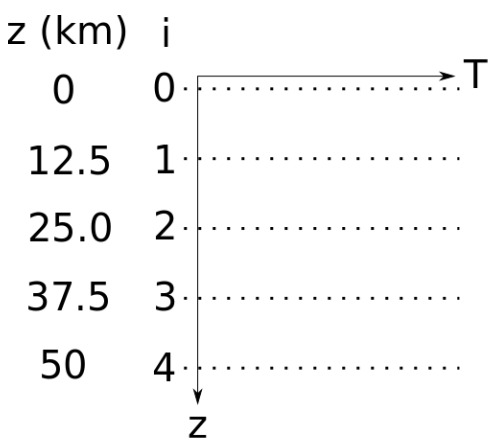
$$T_1 = (q/k)(z_1 - z_0) + T_0$$

$$T_2 = (q/k)(z_2 - z_1) + T_1$$

$$\vdots$$

Example 1: FDM for heat flow

$$T_i = \frac{q}{k}(z_i - z_{i-1}) + T_{i-1}$$



$$T_0 = (q/k)(z_0 - z_{-1}) + T_{-1} \qquad i = -1$$

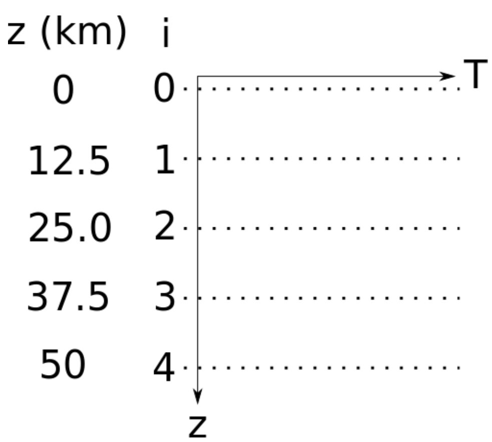
$$T_1 = (q/k)(z_1 - z_0) + T_0$$

$$T_2 = (q/k)(z_2 - z_1) + T_1$$

$$\vdots$$

Example 1: FDM for heat flow

$$T_i = \frac{q}{k}(z_i - z_{i-1}) + T_{i-1}$$



$$T_0 = T_{\mathrm{surf}}$$

$$T_1 = (q/k)(z_1 - z_0) + T_0$$

$$T_2 = (q/k)(z_2 - z_1) + T_1$$

$$\vdots$$

–> Solvable when T_{surf} is known and heat flow *q* is constant and known

`-> heat_flow.py`

Example 1: FDM for heat flow

- Open `Lessons / 05-Finite-differences / scripts / heat_flow.py` in IDLE
- Modify the script at line 42
  - `T[i] = ????`

  and make it use the formula on previous slide to calculate value T_i
- Run (F5) to see if results are what you would expect

Example 2: Steady state heat eq with radiogenic heating

$$0 = k\frac{\mathrm{d}^2 T}{\mathrm{d}z^2} + A$$

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$$0 = k\left(\frac{\left.\frac{\mathrm{d}T}{\mathrm{d}z}\right|_{z=z_i} - \left.\frac{\mathrm{d}T}{\mathrm{d}z}\right|_{z=z_{i-1}}}{z_i - z_{i-1}}\right) + A \qquad z_i - z_{i-1} = \Delta z \quad i = 0, 1, 2, \ldots$$

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$$0 = k\left(\frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta z^2}\right) + A$$

Example 2: Steady state heat eq with radiogenic heating

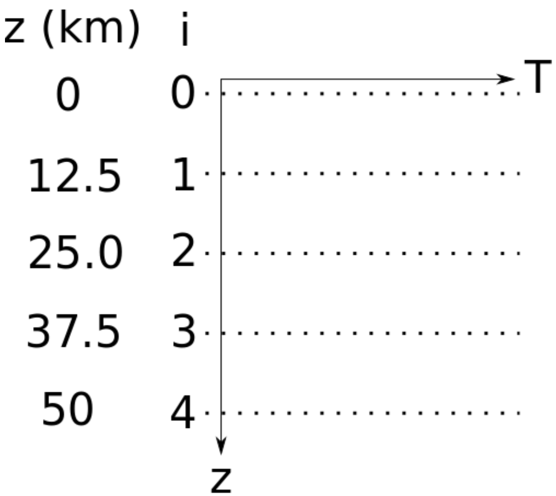
$$0 = k\left(\frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta z^2}\right) + A$$

rewrite:

$$0 = k\left(\frac{T_i - 2T_{i-1} + T_{i-2}}{\Delta z^2}\right) + A$$

rearrange:

$$T_i = -\frac{A}{k}\Delta z^2 + 2T_{i-1} - T_{i-2}$$



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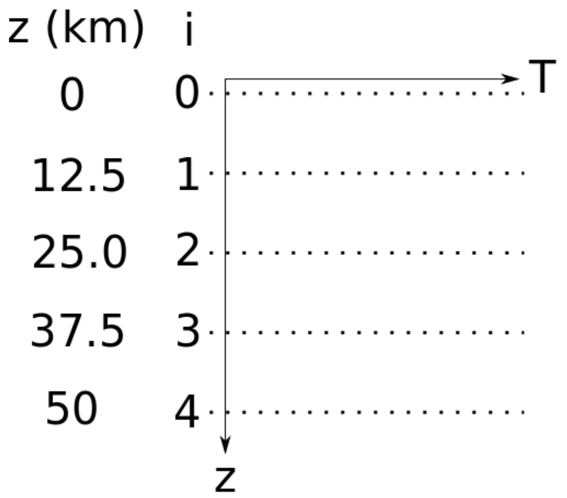

→ Point i = 1 cannot be calculated
→ Can we just assign T_1 a value like we did for T_0?

No? Why not?
Yes? How?

→ `geotherm_with_A.py`

Example 2: Steady state heat eq with radiogenic heating

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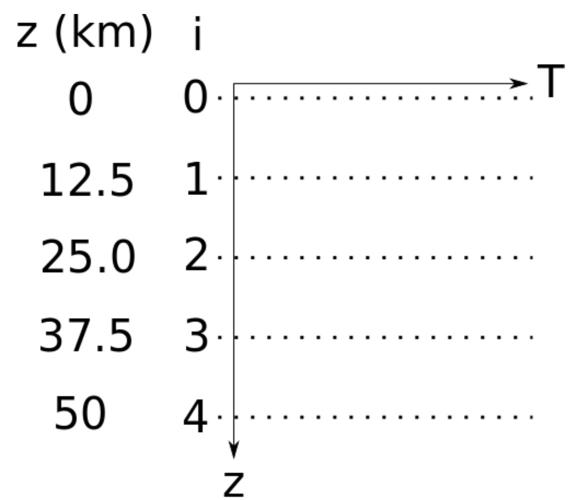

→ `geotherm_with_A.py`

$$T_1 = -\frac{A}{k}\Delta z^2 + 2T_0 - T_{-1}$$

"ghost point"

Example 2: Steady state heat eq with radiogenic heating

→ `geotherm_with_A.py`

Fill in lines with “????”: use equation below to calculate temperature for grid point 1 and for grid points >1

$$T_i = -\frac{A}{k}\Delta z^2 + 2T_{i-1} - T_{i-2}$$

The temperature value at the ghost point has already been calculated. Make sure you understand the logic behind it, and then use it to calculate the temperature value at grid point 1.

Example 2: Steady state heat eq with radiogenic heating

→ `geotherm_with_A.py`

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The temperature value at the ghost point has already been calculated. Make sure you understand the logic behind it, and then use it to calculate the temperature value at grid point 1.

$$T_1 = -\frac{A}{k}\Delta z^2 + 2T_0 - T_{-1}$$

“ghost point”

Example 2: Steady state heat eq with radiogenic heating

- We have an analytical solution for this problem (`Lesson 03 → plot_steady_state_heat_eq_innerbnd.py`)

➔ How accurate is our numerical solution? (`geotherm_with_A_compared.py`)

  ➔ Vary the number of grid points (= grid resolution)

Example 2b: Steady state heat eq with varying radiogenic heating

- What if A=A(z)?

$$0 = k\frac{\mathrm{d}^2T}{\mathrm{d}z^2} + A \quad \rightarrow \quad 0 = k\frac{\mathrm{d}^2T}{\mathrm{d}z^2} + A(z)$$

Example 2b: Steady state heat eq with varying radiogenic heating

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$$0 = k\frac{\mathrm{d}^2T}{\mathrm{d}z^2} + A \quad \rightarrow \quad 0 = k\frac{\mathrm{d}^2T}{\mathrm{d}z^2} + A(z)$$

$$T_i = -\frac{A_i}{k}\Delta z^2 + 2T_{i-1} - T_{i-2}$$

➔ `geotherm_with_A_variable.py`

Example 3: Transient heat equation

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

$$\frac{T^j - T^{j-1}}{t^j - t^{j-1}} \qquad \kappa \left(\frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta z^2} \right)$$

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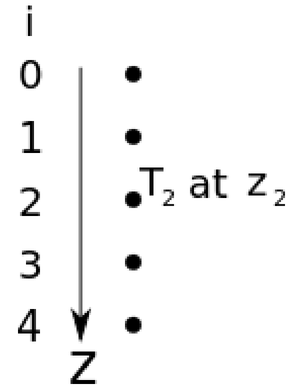

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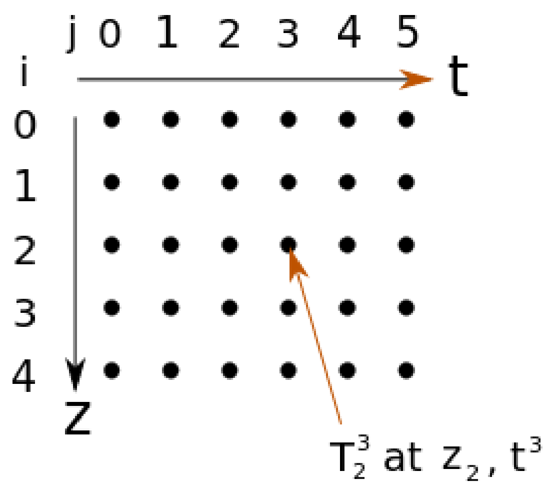

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$$\frac{T_i^j - T_i^{j-1}}{\Delta t} = \kappa \left(\frac{T_{i+1}^{j-1} - 2T_i^{j-1} + T_{i-1}^{j-1}}{\Delta z^2} \right)$$

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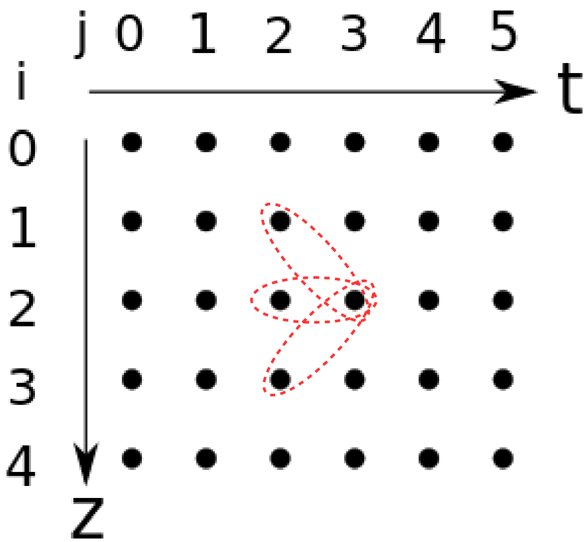

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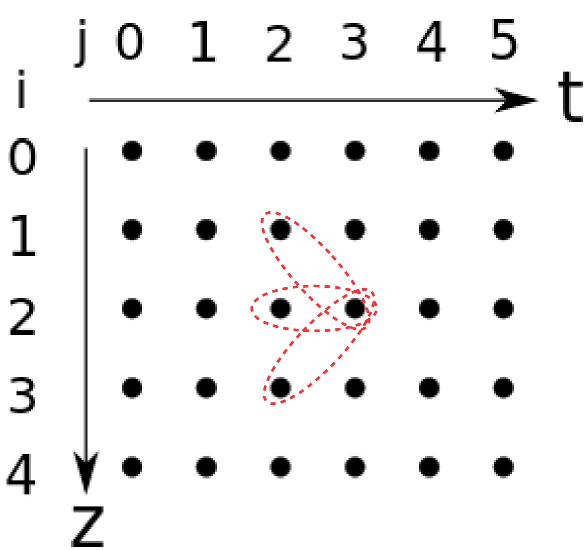

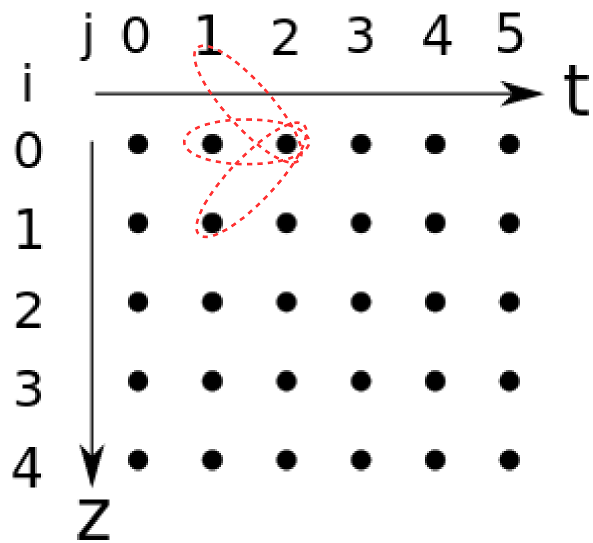

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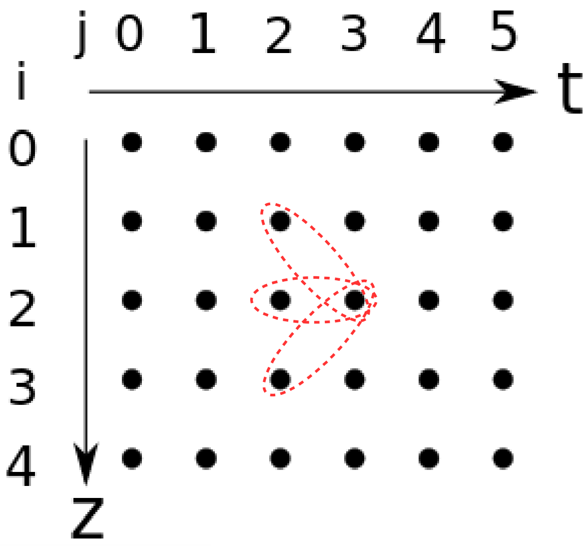

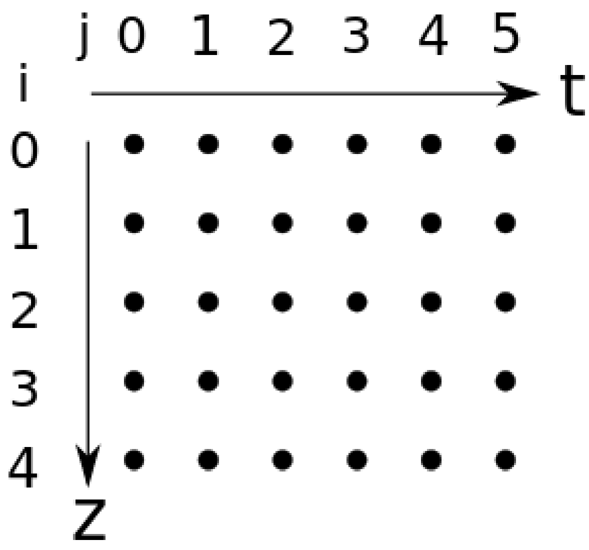

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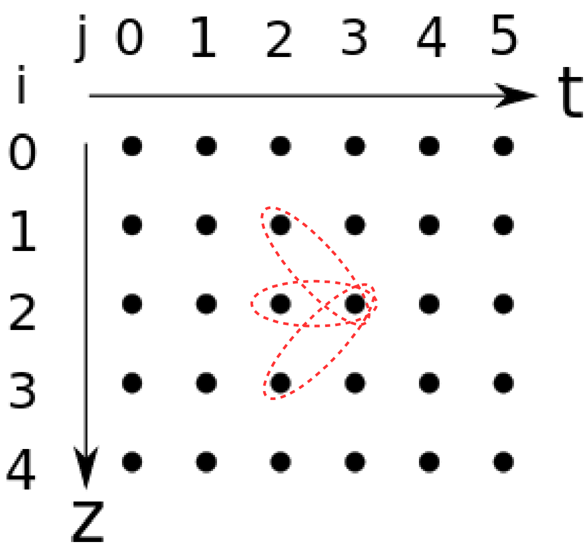

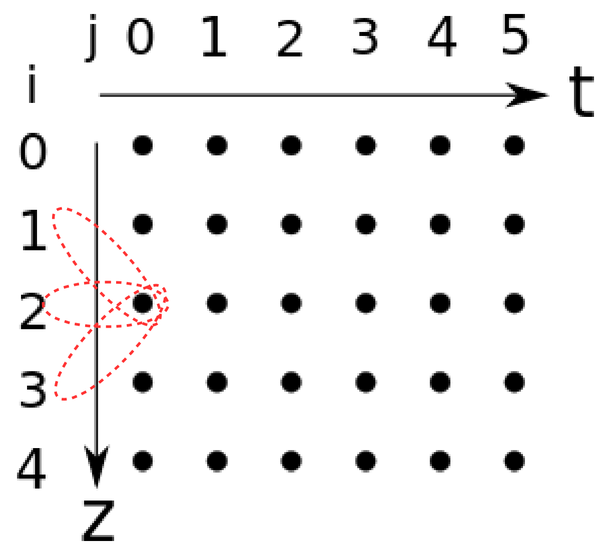

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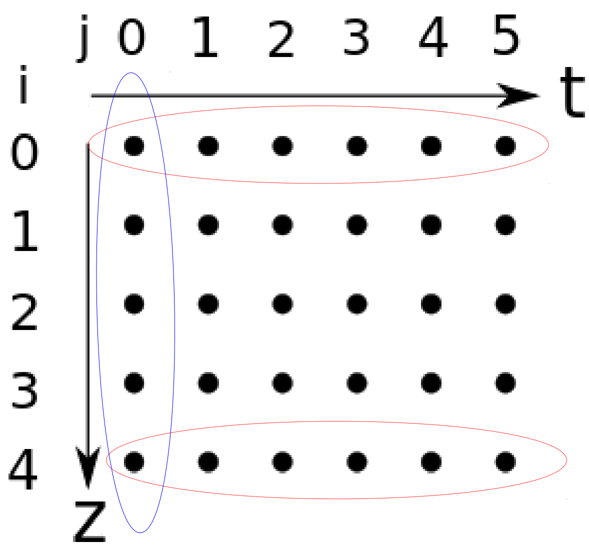


Boundary conditions

Initial conditions

-> heat_transient.py

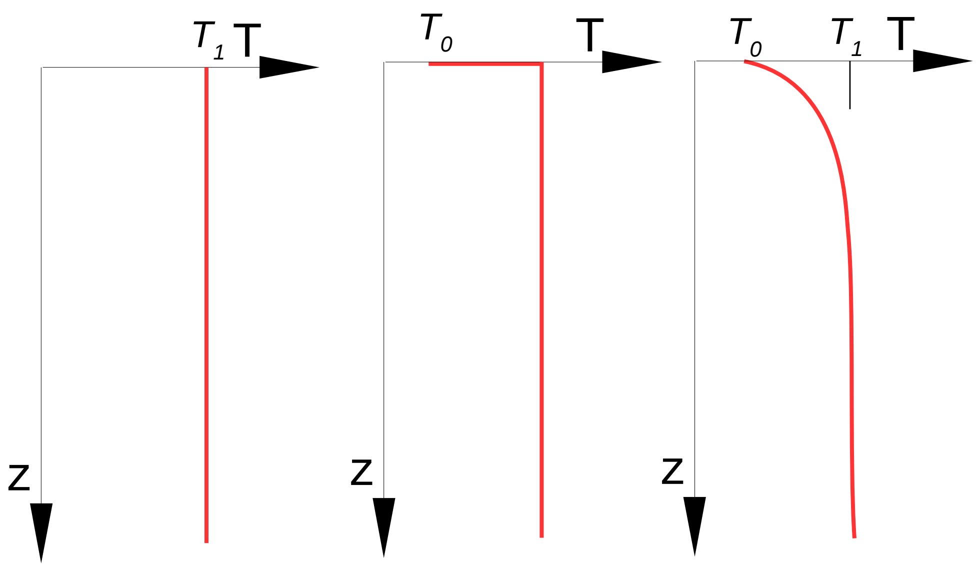
- implement boundary conditions
- implement calculation of the inner grid points

Example 3: Transient heat equation

```
-> heat_transient.py
```

- implement boundary conditions
- implement calculation of the inner grid points

Cooling of oceanic lithosphere:



T_1 = 1300ºC, cools instantly to
T_0 = 0ºC at the surface (sea floor)

T_{surf} = 0ºC
T_{bott} = 1300ºC

$$\frac{T - T_1}{T_0 - T_1} = \mathrm{erfc}\frac{z}{2\sqrt{\kappa t}}$$

Stability of heat diffusion in FDM

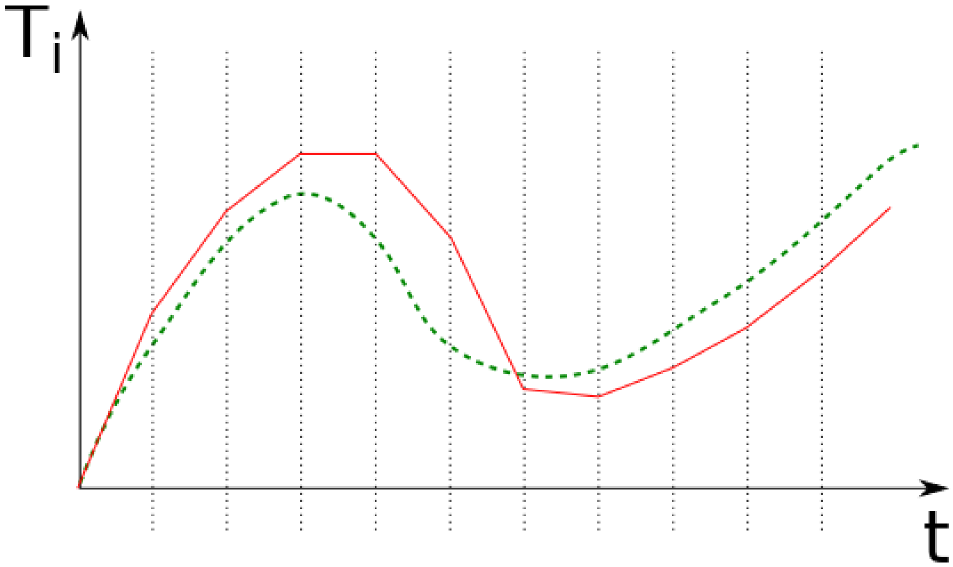
```
-> heat_transient.py
```

- increase time step size, e.g.

```
dt = 1.0 * 112500000000000.0
dt = 1.2 * 112500000000000.0
dt = 2.0 * 112500000000000.0
```

- What happens? Why?

$$T_i^j = \kappa \left(\frac{T_{i+1}^{j-1} - 2T_i^{j-1} + T_{i-1}^{j-1}}{\Delta z^2} \right) \Delta t + T_i^{j-1}$$



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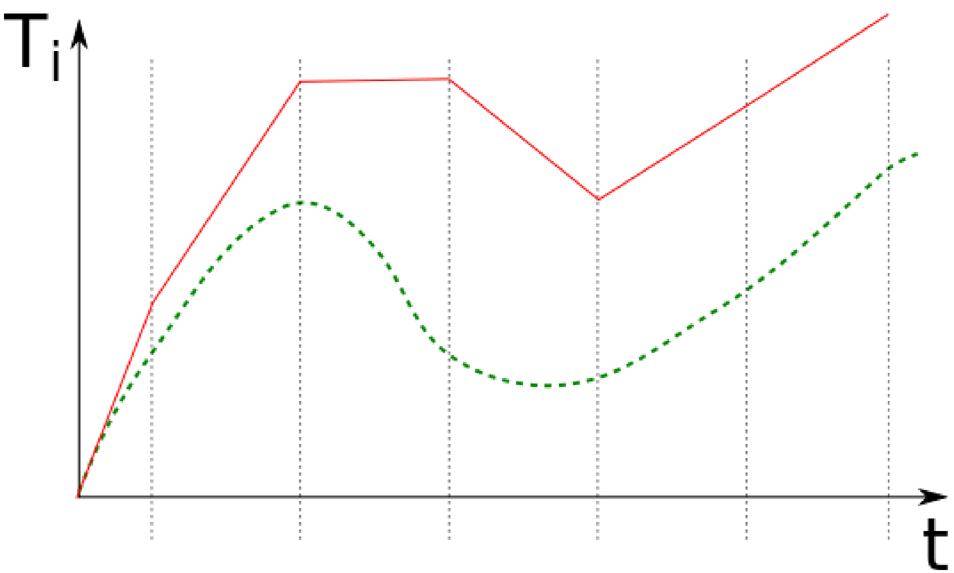

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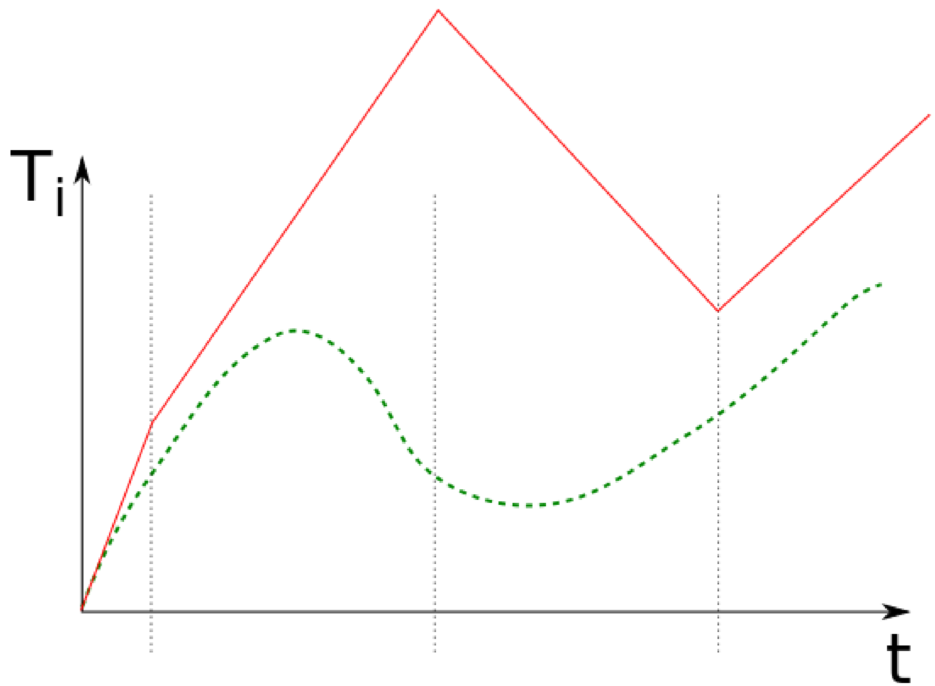

Stability of heat diffusion in FDM

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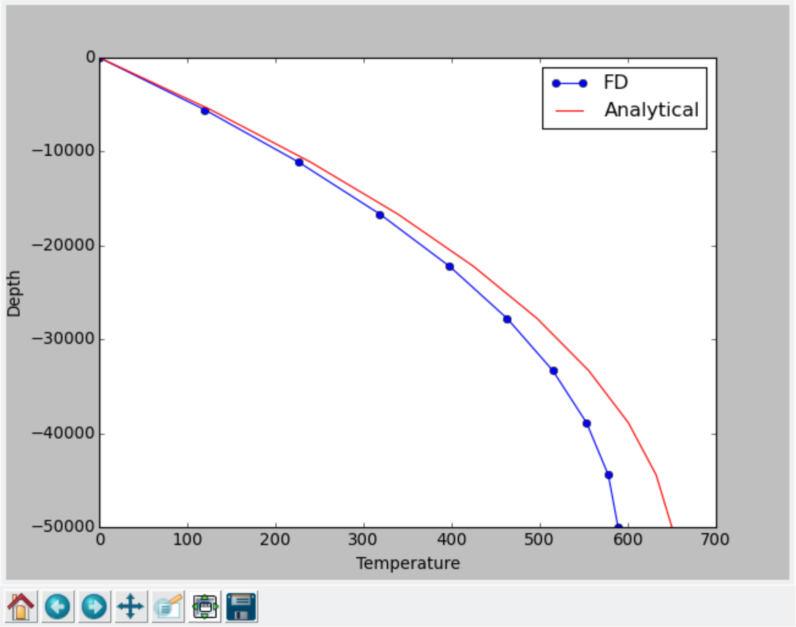
The numerical scheme only allows heat to diffuse one grid space to the next grid point

… but the sum of temperatures in surrounding grid points is multiplied by d*t* → too large d*t* can make $T_1 > T_2$ even if originally $T_1 < T_2$ → heat diffuses "upstream" – should not be possible!

von Neumann stability analysis → $$\Delta t \leq \frac{\Delta x^2}{2\kappa}$$

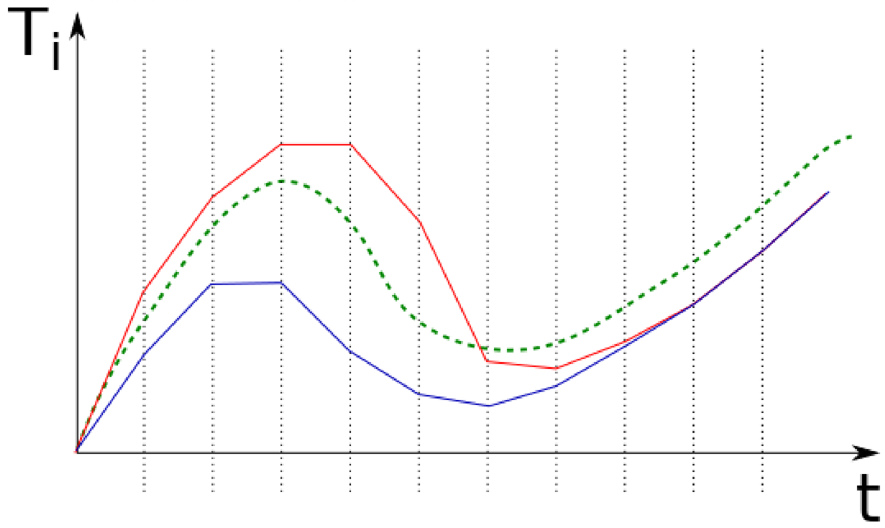
Stability of heat diffusion in FDM

von Neumann **stability** analysis → $\Delta t \leq \dfrac{\Delta x^2}{2\kappa}$



$$\text{stability} \neq \text{accuracy}$$

Time stepping schemes in finite differences



Forward Euler
Backward Euler

Overshoots
Undershoots

Explicit
Implicit

Stability criterion
Always stable

$$T_i^j = \kappa \left(\frac{T_{i+1}^{j-1} - 2T_i^{j-1} + T_{i-1}^{j-1}}{\Delta z^2} \right) \Delta t + T_i^{j-1}$$

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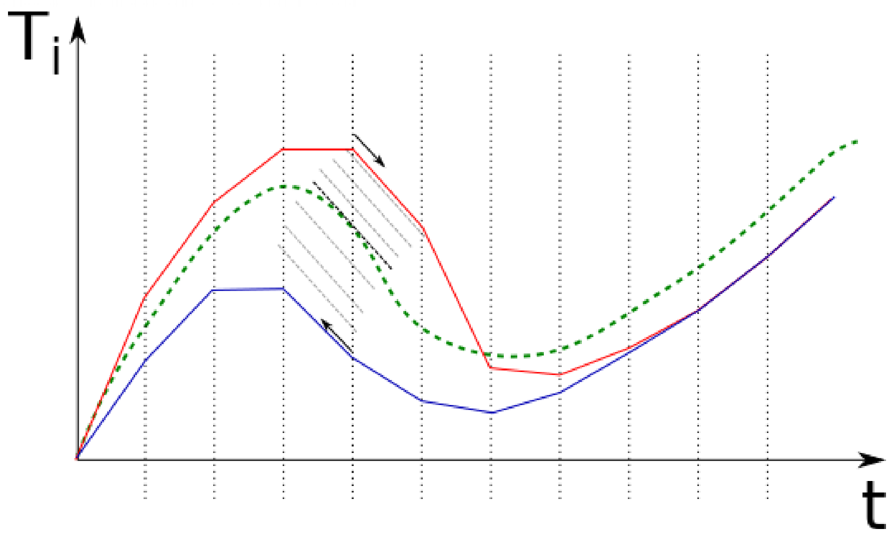

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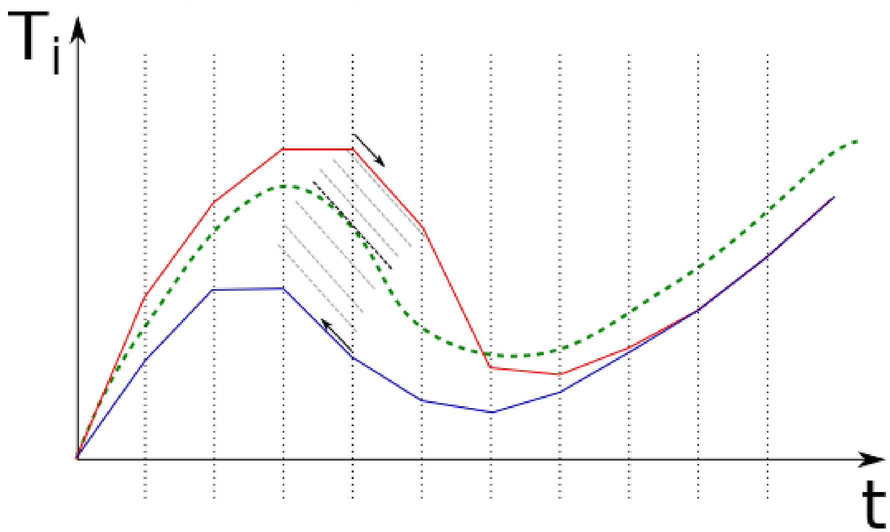

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Averaging schemes,
e.g. Crank-Nicolson

Heat equation, implicit (backward Euler) time stepping scheme

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Heat equation, implicit (backward Euler) time stepping scheme

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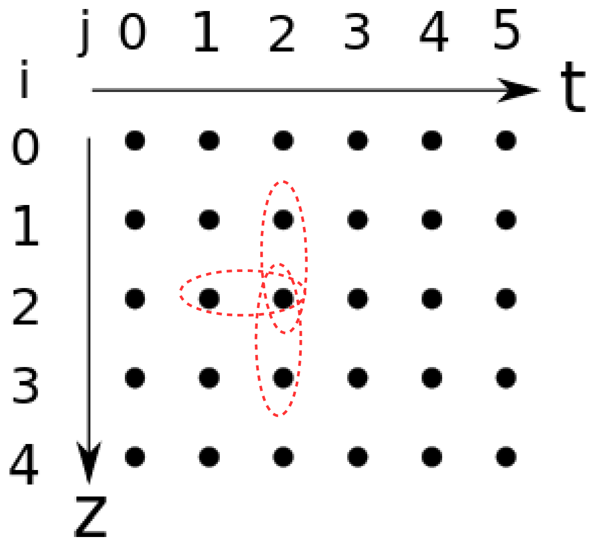

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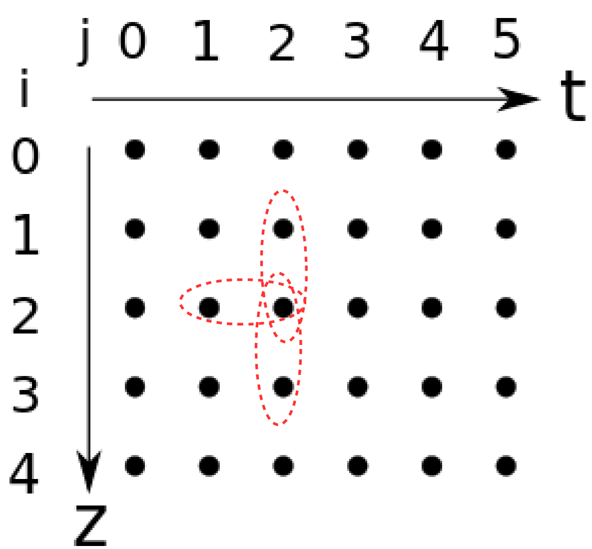


$$T_0^2 = T_{\text{bnd}}$$

$$T_1^2 = \kappa \left(\frac{T_2^2 - 2T_1^2 + T_0^2}{\Delta z^2} \right) \Delta t + T_1^1$$

$$T_2^2 = \kappa \left(\frac{T_3^2 - 2T_2^2 + T_1^2}{\Delta z^2} \right) \Delta t + T_2^1$$

$$\vdots$$

→ System of linear equations (n unknowns, n equations, n = number of grid points)

FDM for flow mechanics

$$\frac{\partial p}{\partial x} = \eta \frac{\partial^2 u}{\partial y^2}$$

$$\tau = \eta \frac{\mathrm{d}u}{\mathrm{d}y}$$

$$\eta \frac{\partial^2 u}{\partial y^2} - P_{drop} = 0$$

$$\eta \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta y} - P_{drop} = 0$$

$$u = \mathrm{const.}$$ "Dirichlet" **no-slip**

$$\frac{\partial u}{\partial y} = 0 \Rightarrow \frac{u_i - u_{i-1}}{\Delta y} = 0$$ "von Neumann" **free-slip**

Why use FDM (or any numerical method)

- 1D → 2D/3D
  - Analytical solutions very complicated
  - Numerical solutions longer to type but still only +, -, *, and /

$$T_{i,h}^{j} = \kappa \left(\frac{T_{i+1,h}^{j} - 2T_{i,h}^{j} + T_{i-1,h}^{j}}{\Delta z^2} + \frac{T_{i,h+1}^{j} - 2T_{i,h}^{j} + T_{i,h-1}^{j}}{\Delta x^2} \right) \Delta t + T_{i,h}^{j-1}$$

Why use FDM (or any numerical method)

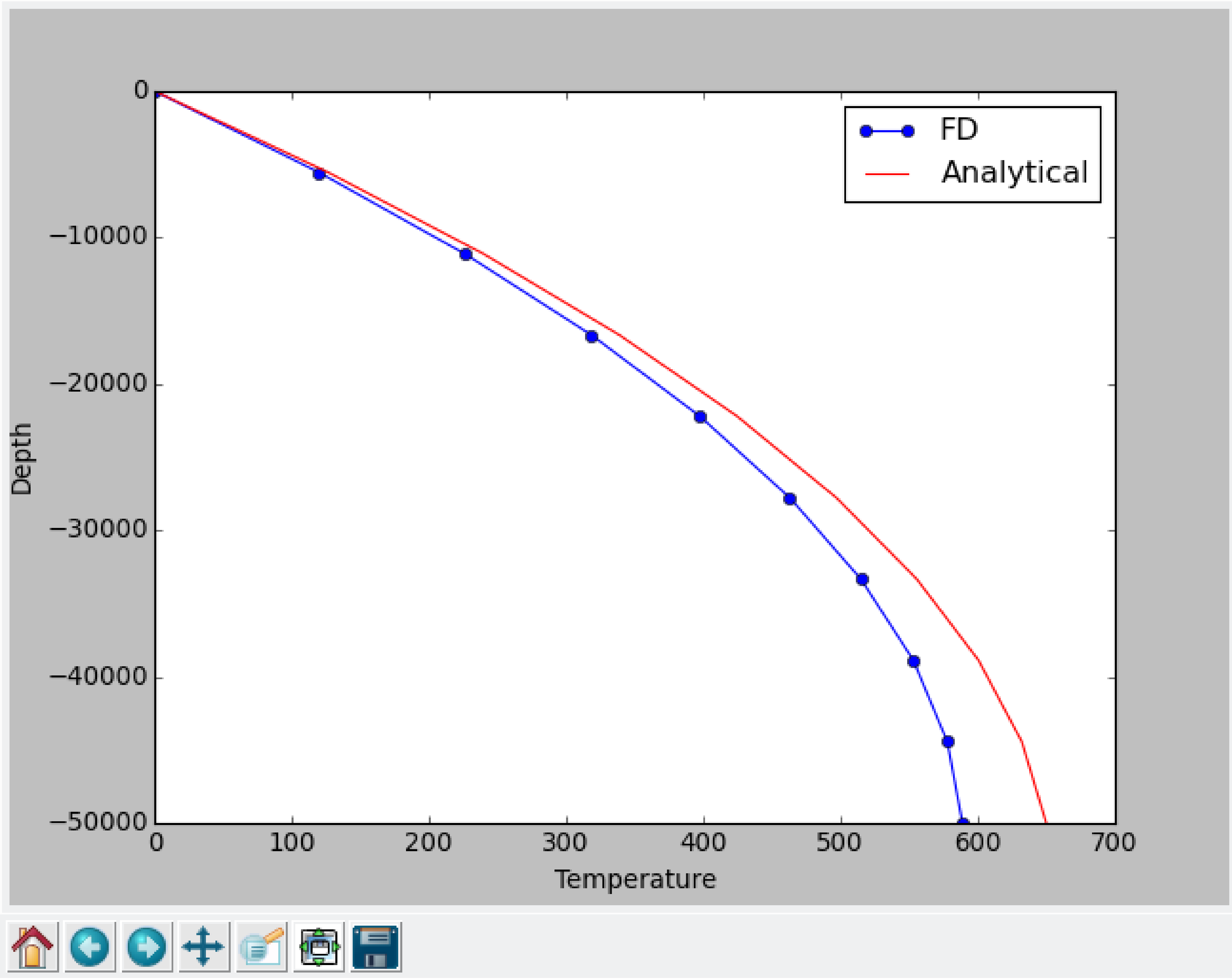
- Complex geometries, e.g. spatially varying material parameters or deformed model boundaries
  - Longer, no more or only slightly more complex

$$T_i^j = \left(\frac{k_{i+\frac{1}{2}} \frac{T_{i+1}-T_i}{\Delta z} - k_{i-\frac{1}{2}} \frac{T_i - T_{i-1}}{\Delta z}}{\Delta z} \right) \rho_i C_{p,i} \Delta t + T_i^{j-1} \; ; \quad k = k(z), \; \rho = \rho(z), \; C_p = C_p(z)$$

- A bit more complexity involved in non-linear cases
  - e.g. k=k(T)
    - ➔ Iterative solutions
  - Still virtually always superior to analytical approach

Why NOT use FDM (or any numerical method)

- In complex (read: typical) model set-ups accuracy is hard to estimate
  - ➔ Resolution tests
    - Error in FD of heat equation is proportional to Δt and Δx^2 ("first order accurate in time", "second order accurate in space")
  - ➔ Benchmarks


FD
Analytical
Depth
Temperature
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200
300
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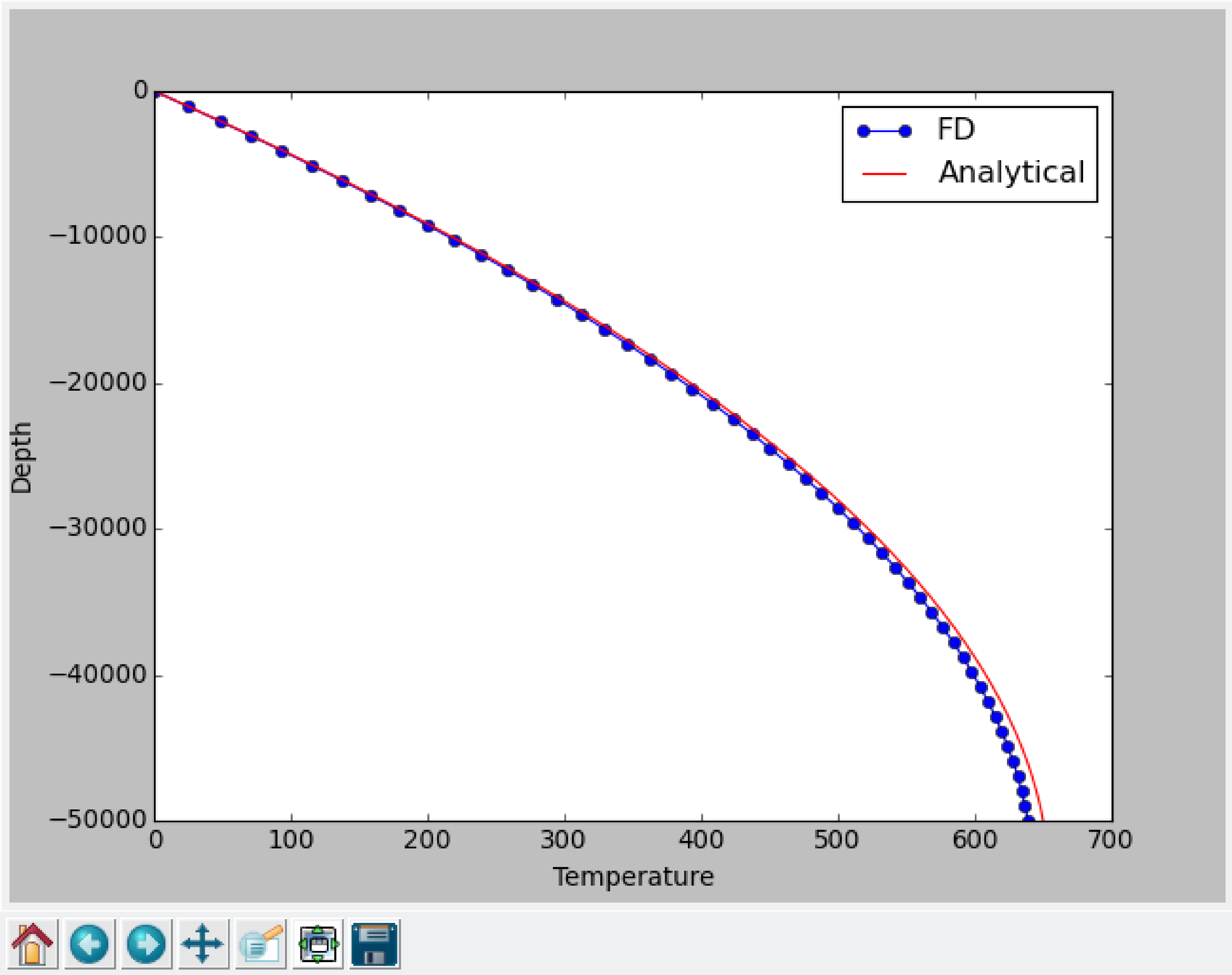

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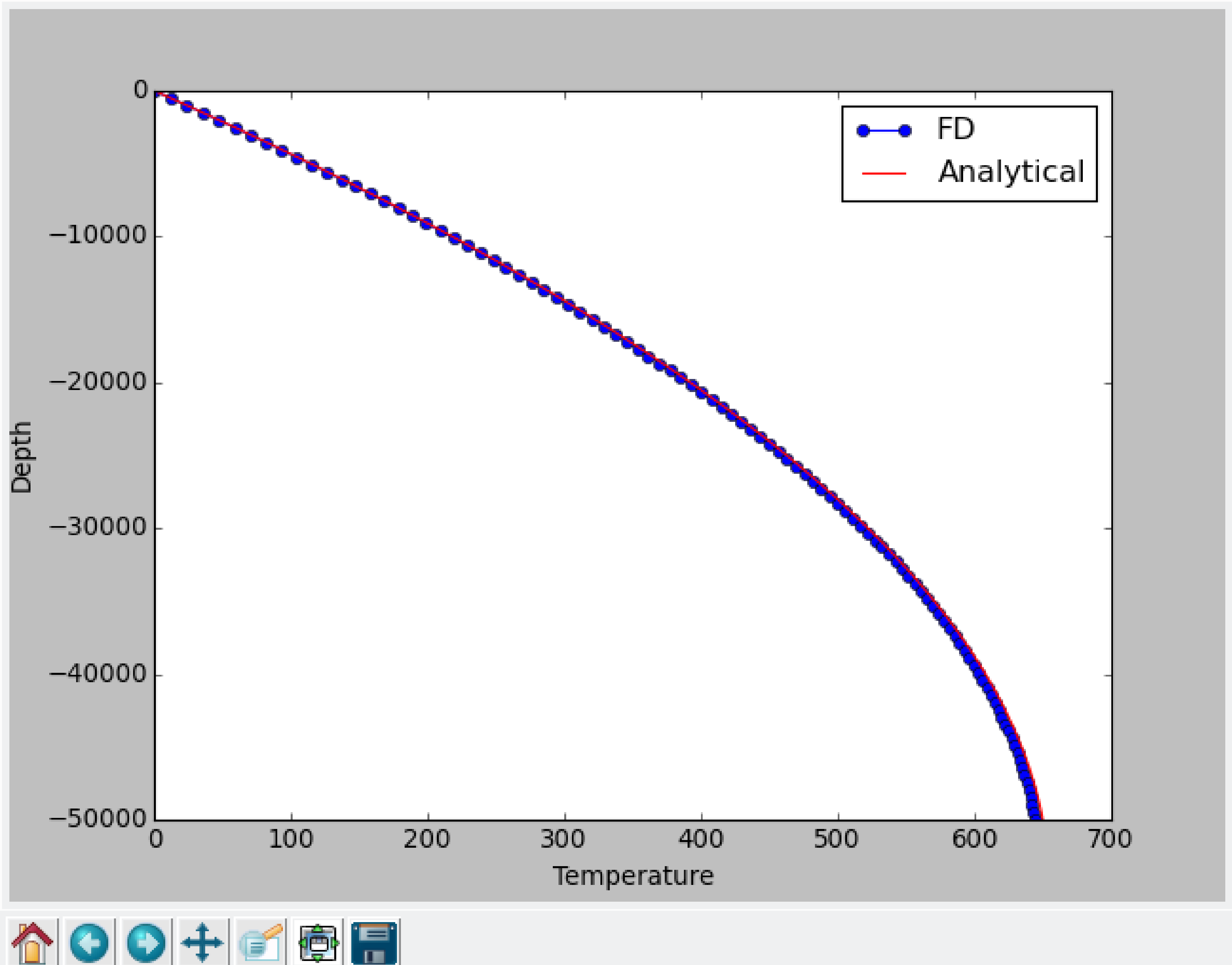

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