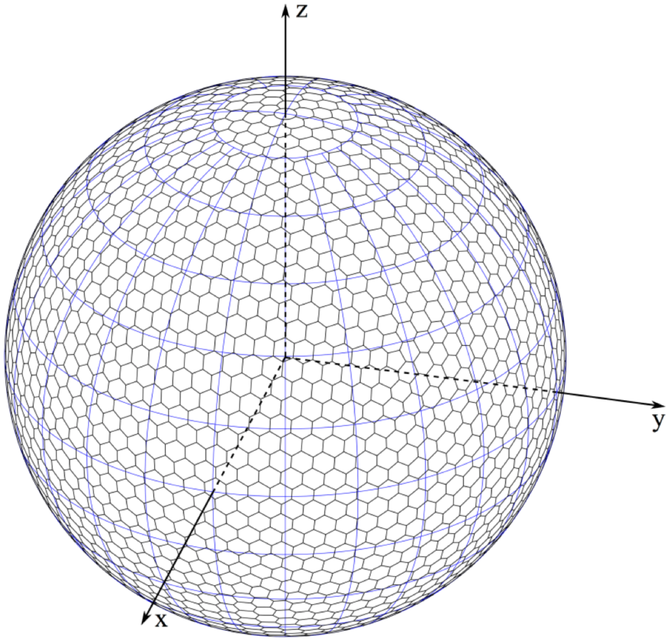
INTRODUCTION TO FINITE-VOLUME DISCRETIZATION

Timothy Chui

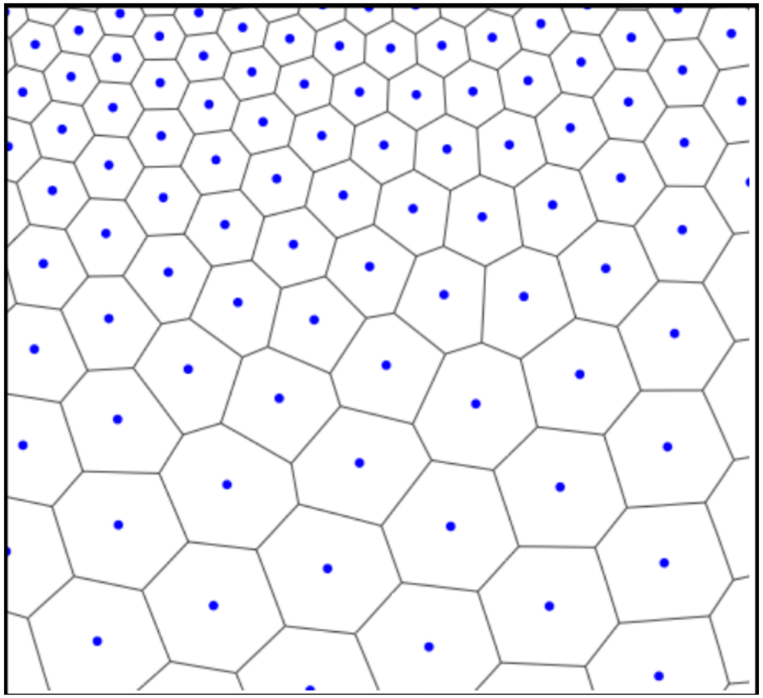
Mar. XX, 2019



http://mpas-dev.github.io/atmosphere/tutorial.html

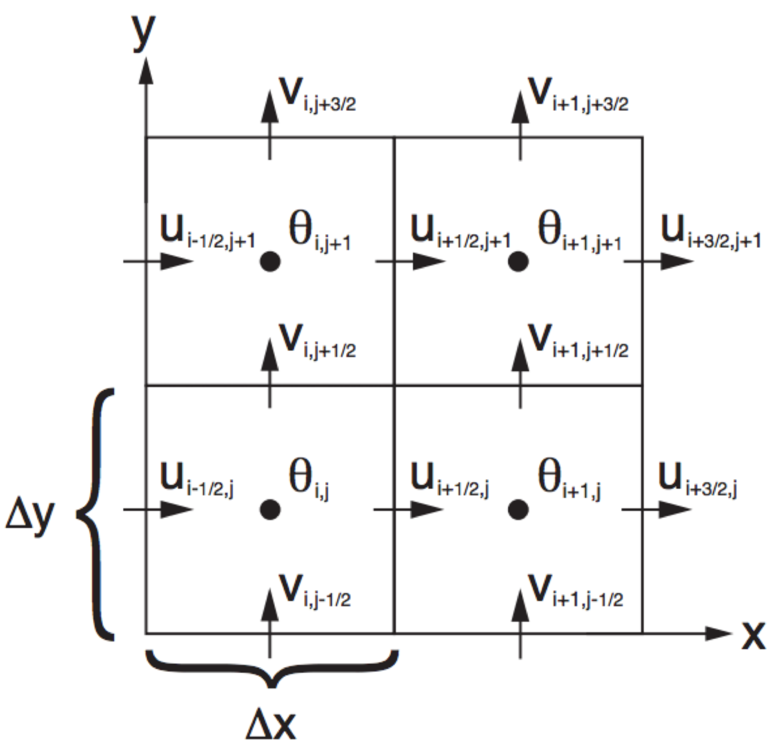
Overview of seminar series

- Introduction to MPAS
- The MPAS Mesh
- **Introduction to Finite-Volume Discretization**
- MPAS Numerics and Dynamics
- **MPAS Workshop

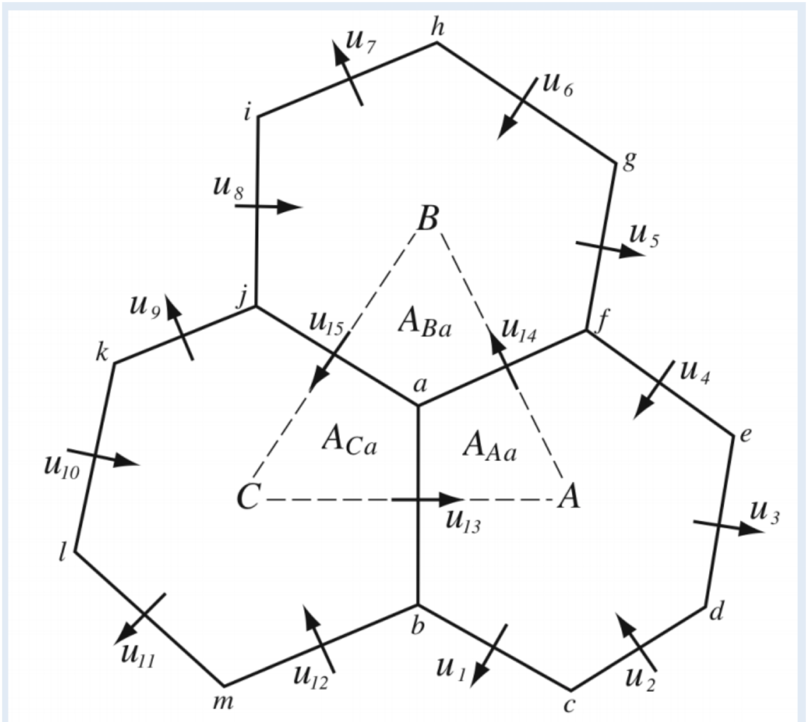


http://mpas-dev.github.io/atmosphere/tutorial.html

WRF vs. MPAS Discretization



horizontal grid

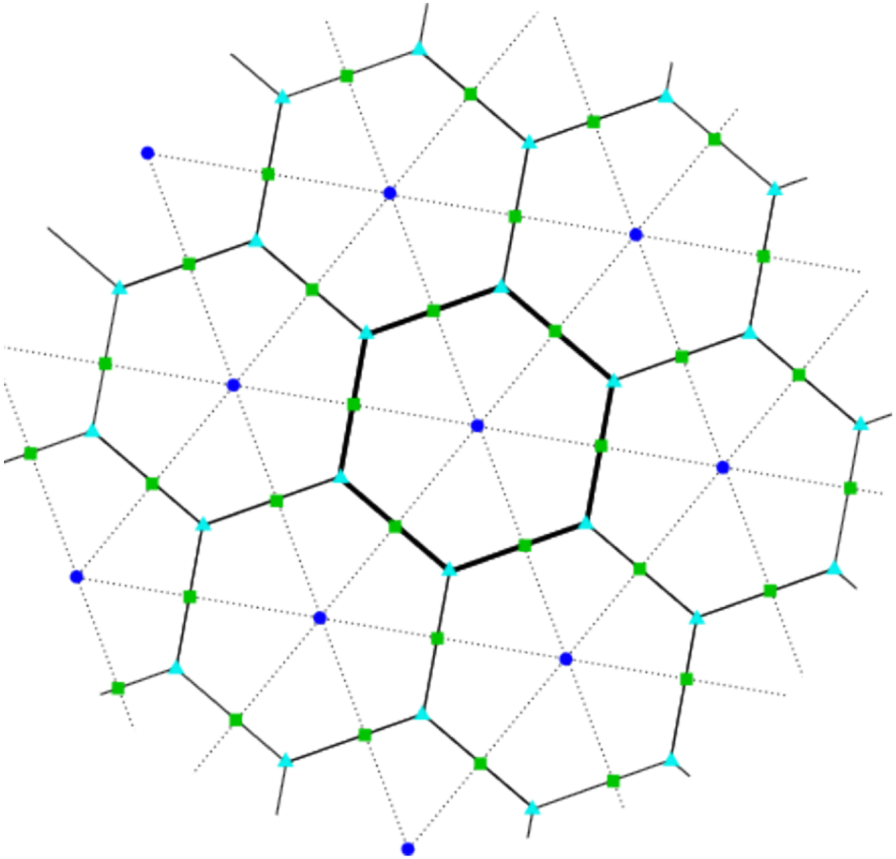


http://mpas-dev.github.io/atmosphere/tutorial.html

- Eulerian, finite-difference, **structured**
- Eulerian, finite-volume, **unstructured**

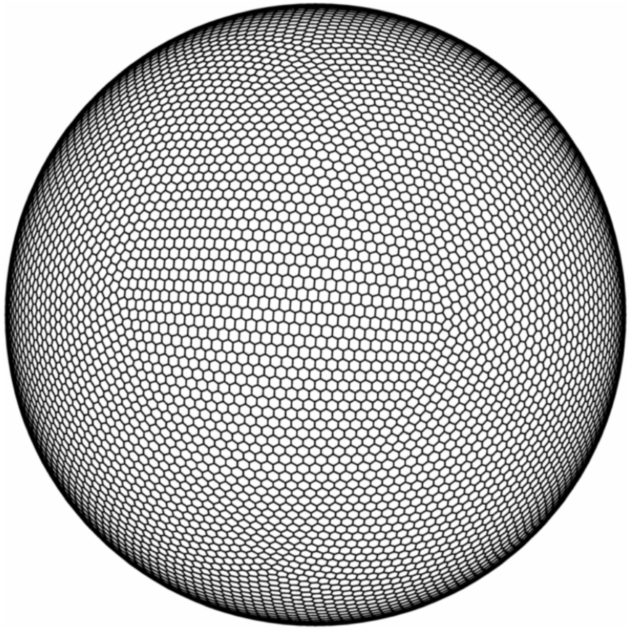
Table of Contents

- Why finite-volume (FV)?
- 1D Advection Equation
- Review of finite-difference (FD) discretization
- Introduction to FV discretization
- Summary



http://mpas-dev.github.io/atmosphere/tutorial.html

Why FV Discretization?



http://mpas-dev.github.io/atmosphere/tutorial.html

- Easy to conserve mass, momentum and energy (“what comes in must go out”)
- Easy (compared to FD) for use on unstructured meshes and weird meshes
- Used by engineers to handle shockwaves and transconic flow
- Used to handle growth of nonlinear quantities like potential enstrophy and total energy (Arakawa 1966)
    - Better than FD for handling shock waves

Arakawa (1966)
Ringler et al. (2011)

FV in a Nutshell

https://www.convertwithcontent.com/web-marketing-in-a-nutshell/

- Work with boxes instead of points
- Figure out what comes in (**fluxes in**) and goes out (**fluxes out**) of the boxes
- Sum all that up, call it the **flux integral**
- Don't forget about source/sink terms ("physics") within each box
- ^Take all of that, average over each box = **control-volume average**

Aside…flux-form equations

Using the variables defined above, the flux-form Euler equations can be written as

$$\partial_t U + (\nabla \cdot \mathbf{V} u) - \partial_x(p\phi_\eta) + \partial_\eta(p\phi_x) = F_U \quad (2.3)$$

$$\partial_t V + (\nabla \cdot \mathbf{V} v) - \partial_y(p\phi_\eta) + \partial_\eta(p\phi_y) = F_V \quad (2.4)$$

$$\partial_t W + (\nabla \cdot \mathbf{V} w) - g(\partial_\eta p - \mu) = F_W \quad (2.5)$$

$$\partial_t \Theta + (\nabla \cdot \mathbf{V}\theta) = F_\Theta \quad (2.6)$$

$$\partial_t \mu + (\nabla \cdot \mathbf{V}) = 0 \quad (2.7)$$

$$\partial_t \phi + \mu^{-1}[(\mathbf{V} \cdot \nabla\phi) - gW] = 0 \quad (2.8)$$

$$\boldsymbol{V = \mu v, \mu = \text{“mass”} = p_{surface} - p_{top}}$$

Skamarock et al. (2008)

Aside…flux-form equations

$$\frac{\partial \mu v}{\partial y} = v\frac{\partial \mu}{\partial y} + \mu\frac{\partial v}{\partial y}$$

Aside…flux-form equations

$$\frac{\partial \mu v}{\partial y} \approx \frac{(\mu v)_i - (\mu v)_{i-1}}{\Delta y}$$

$$v\frac{\partial \mu}{\partial y} + \mu\frac{\partial v}{\partial y} \approx v_i\frac{\mu_i - \mu_{i-1}}{\Delta y} + \mu_i\frac{v_i - v_{i-1}}{\Delta y}$$

1D Advection Equation

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

- 1D advection equation
  - “Convection” equation for engineers
- $-\infty \le x \le \infty$

1D Advection Equation

- Initial condition on domain with some function *F(x)*

$$T(x,0) = F(x)$$

- Analytic solution

$$\boxed{T(x,t) = F(x - ut)}$$

1D Advection Equation - Goal

- Find a semi-discrete form for the advection equation

$$\boxed{\frac{\partial T}{\partial t}} + \boxed{u\frac{\partial T}{\partial x}} = 0$$

- Don't handle time derivative; that's dealt with separately (i.e. Forward-Euler, Runge-Kutta 3rd, etc.)

- Discretize space derivative

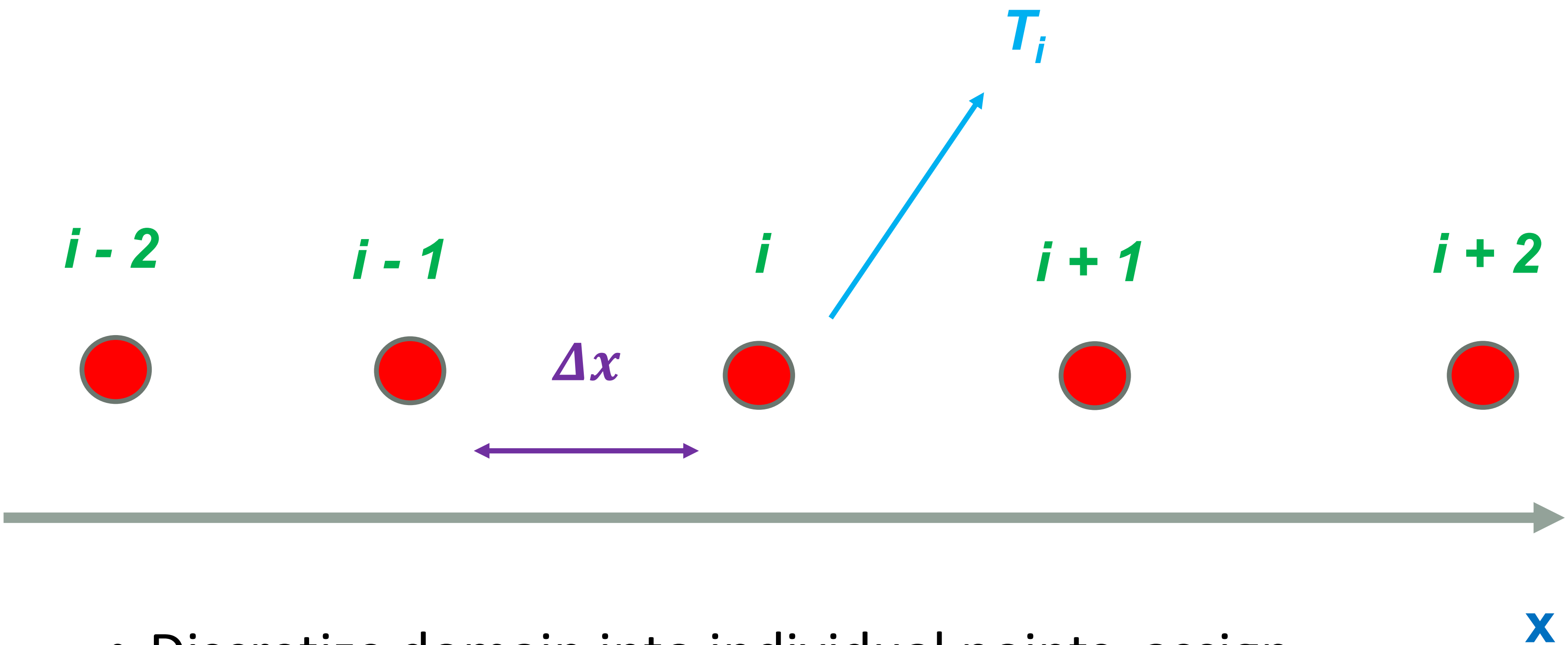
1D Advection Equation - Goal

- Assume $u \geq 0, \text{constant}$ (space + time)
- Superscript n = integration time step

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

$$\frac{\partial T}{\partial t} + u\frac{T_i^n - T_{i-1}^n}{\Delta x} = 0$$

FD Discretization



- Discretize domain into individual points; assign values to each point (i.e. T_i)
- Gradients are calculated by taking finite differences across these points

Taylor…

…Expansion

Taylor Expansion

$$f(x) = f(x_o) + \frac{\partial f(x_o)}{\partial x}(x - x_0) + \frac{\partial^2 f(x_o)}{\partial x^2}\frac{(x - x_0)^2}{2!} + \frac{\partial^3 f(x_o)}{\partial x^3}\frac{(x - x_0)^3}{3!} + \cdots$$

- Evaluate f at points x close to x_o

Taylor Expansion (at *i*)

$$T(x) = T_i + \frac{dT}{dx}\bigg|_i (x - x_i) + \frac{1}{2!}\frac{d^2T}{dx^2}\bigg|_i (x - x_i)^2 + \ldots$$

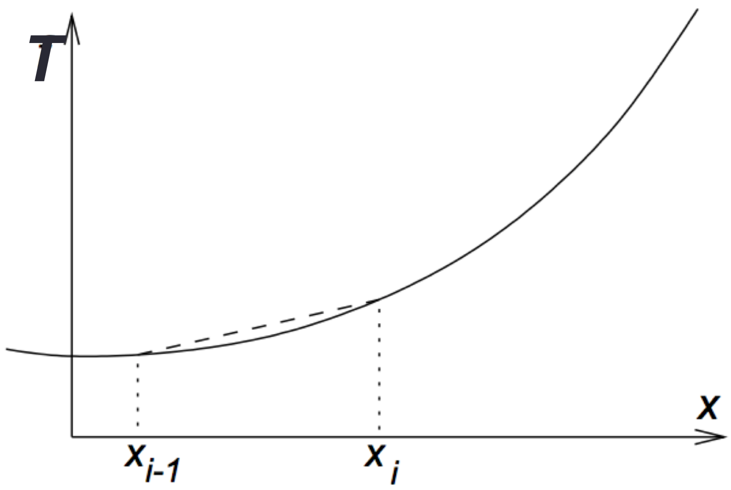
Taylor Expansion (at *i*)

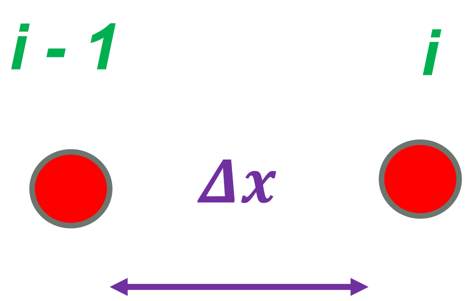
$$T_i = T(x) - \left.\frac{dT}{dx}\right|_i (x - x_i) - \frac{1}{2!}\left.\frac{d^2T}{dx^2}\right|_i (x - x_i)^2 - \ \ldots$$

Taylor Expansion (at *i*)

- Let $x = x_{i-1}$ and $x_i - x_{i-1} = \Delta x$

$$T_i = T_{i-1} + \frac{dT}{dx}\bigg|_i \Delta x + \frac{1}{2!}\frac{d^2T}{dx^2}\bigg|_i \Delta x^2 + \ \ldots$$





http://cfd.mace.manchester.ac.uk/twiki/pub/Main/TimCraftNotes_All_Access/cfd1-findiffs.pdf

Taylor Expansion (at *i*)

- Solve for $\frac{dT}{dx}\Big|_i$

$$\frac{dT}{dx}\Big|_i = \frac{T_i - T_{i-1}}{\Delta x} - \frac{1}{2!}\frac{d^2T}{dx^2}\Big|_i \Delta x + \ldots$$

$$\boxed{\frac{dT}{dx}\Big|_i = \frac{T_i - T_{i-1}}{\Delta x} + \mathcal{O}(\Delta x)}$$

FD Backward Difference

- Semi-discrete form

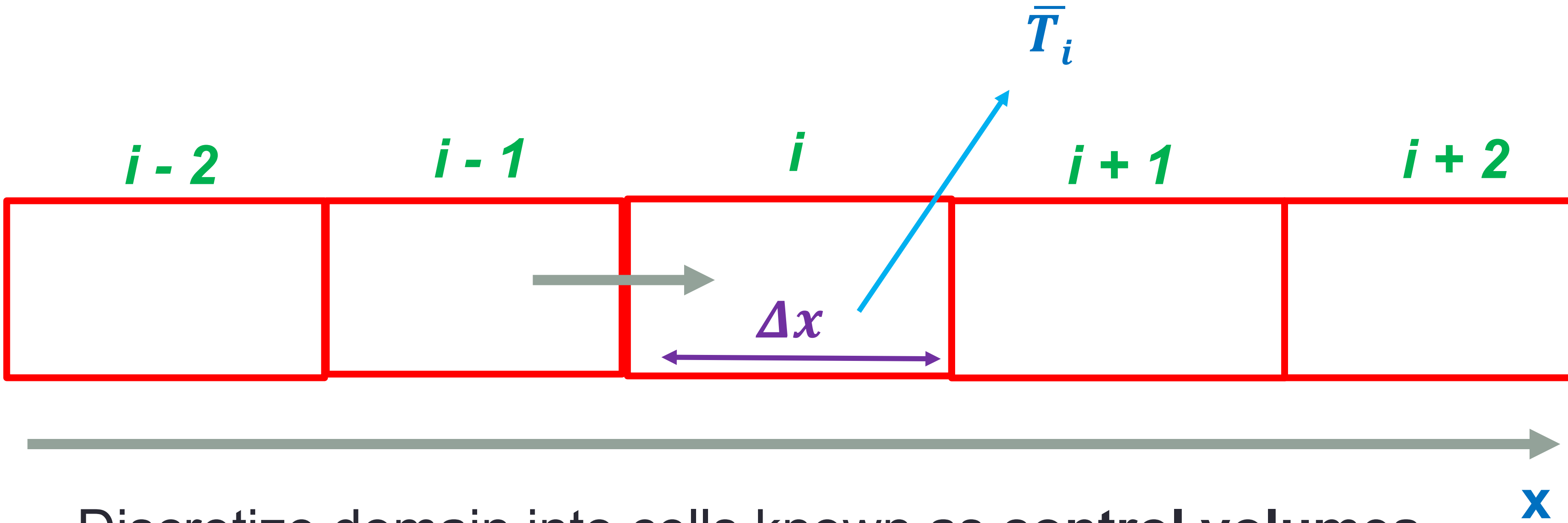
$$\frac{\partial T}{\partial t} + u\frac{T_i^n - T_{i-1}^n}{\Delta x} = 0$$

FD Upwind

- 1st order time, space (explicit)

$$T_i^{n+1} = T_i^n + \Delta t \left(u \frac{T_i^n - T_{i-1}^n}{\Delta x} \right)$$

FV Discretization



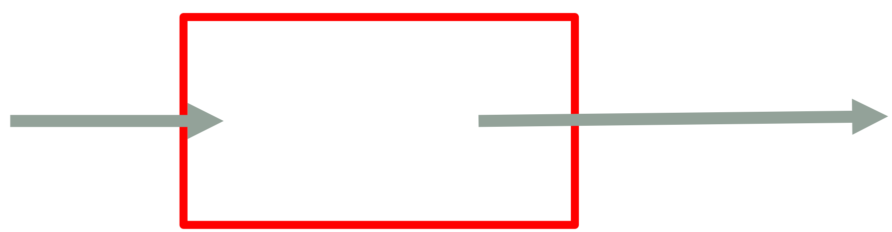
- Discretize domain into cells known as **control volumes** (CVs)
- Assign CV-averaged values to each CV (i.e. $\bar{T}_i$)
- Flux into destination CV = flux out of source CV

FV Discretization

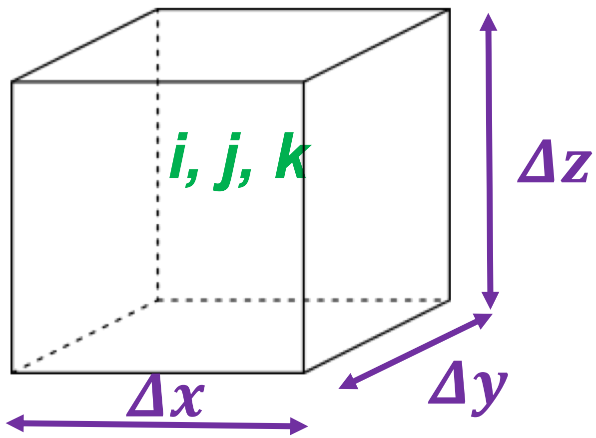
- FV is based on **flux integrals** (i.e. computation of how much "stuff" enters and exits a CV)

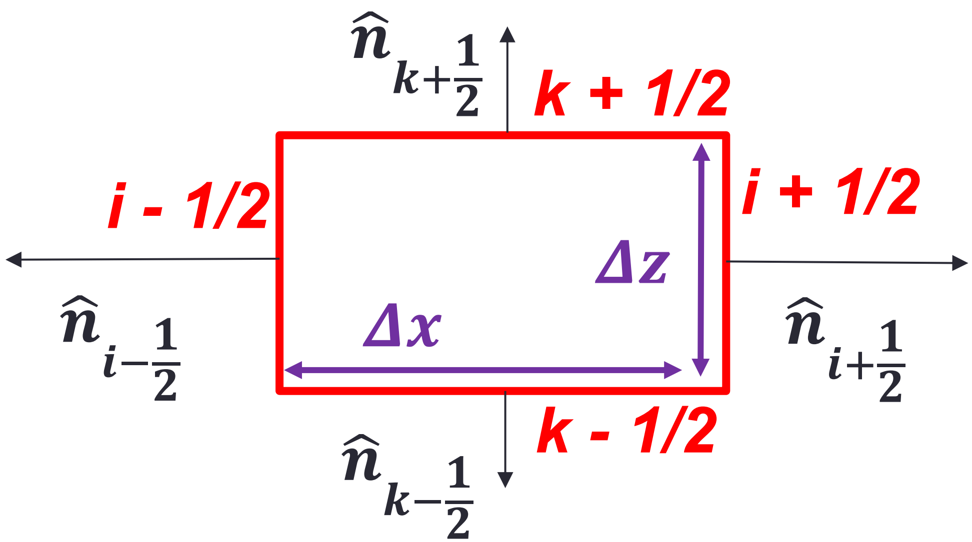
- Goal of FV discretization of a PDE: represent the spatial derivatives in terms of these flux integrals

$$\frac{\partial uT}{\partial x} \approx \text{flux of stuff exiting to the right } - \text{flux of stuff moving in from the left}$$



FV Notation





- Consider 3D **structured** and **fixed** (not moving) **grid**
- $\hat{n}_{i+\frac{1}{2}}$ = unit normal pointing outwards of face *i+1/2*

FV General Derivation

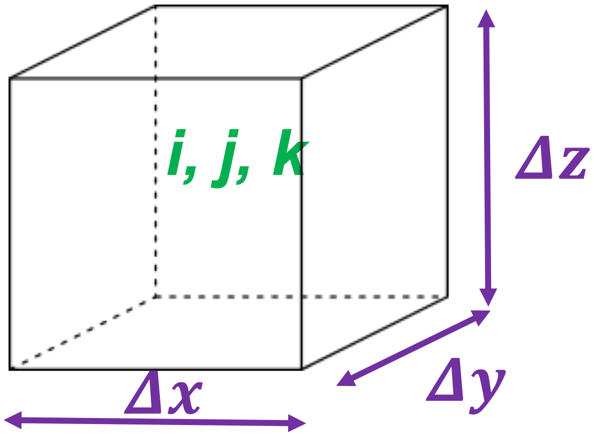
- Some generic PDE
- S = some source term, $\vec{F} = (F, G, H)$; F, G, H can be derivatives

$$\boxed{\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = S}$$

FV General Derivation

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = S$$

- **Express how *U* changes as a CV-averaged value in the box**



FV General Derivation

1) Integrate over control volume CV = $CV_{i,j,k}$

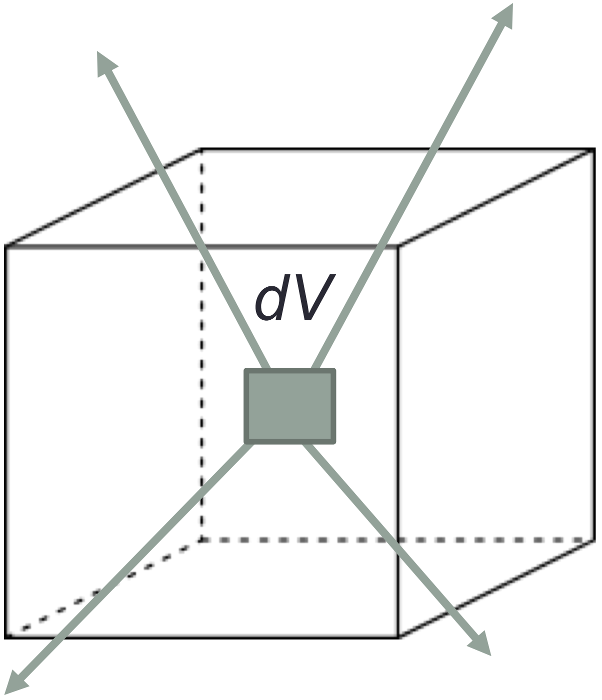
$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = S$$

$$\iiint_{CV} \frac{\partial U}{\partial t} dV + \iiint_{CV} \nabla \cdot \vec{F} \, dV = \iiint_{CV} S \, dV$$

CV = control volume; dV = volume element

FV General Derivation

$$\iiint_{CV} \nabla \cdot \vec{F}\, dV$$



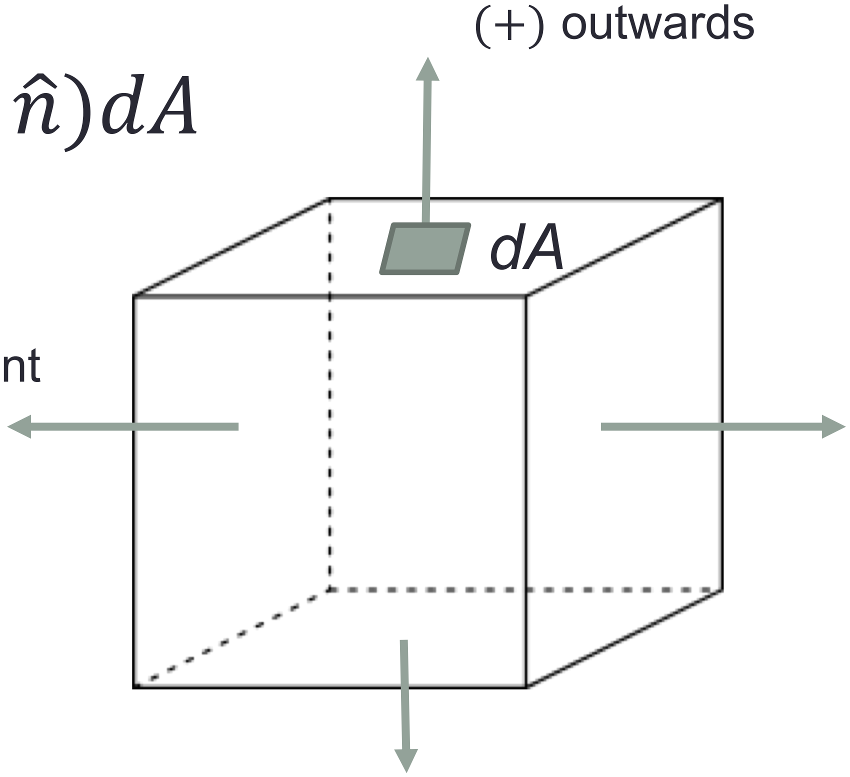
FV General Derivation

- **Divergence (Gauss's) theorem**

$$\iiint_{CV} \nabla \cdot \vec{F}\, dV = \oint\!\!\!\oint_{\partial CV} (\vec{F} \cdot \hat{n})\, dA$$

∂CV = boundary of CV; *dA* = surface element

$$\vec{F} \cdot \hat{n} = F n_x + G n_y + H n_z$$



FV General Derivation

2) Assume CV is fixed (mesh doesn’t change)

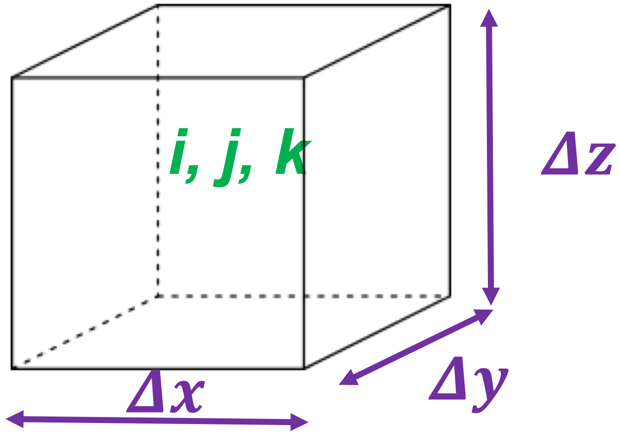
$$\iiint_{CV} \frac{\partial U}{\partial t} dV = \frac{d}{dt} \iiint_{CV} U dV$$

FV General Derivation

3) Define CV average

$$V = \Delta x \Delta y \Delta z$$

$$\overline{U} = \frac{1}{V} \iiint_{CV} U dV$$



$$\bar{S} = \frac{1}{V} \iiint_{CV} S dV$$

FV General Derivation

4) Divide through by *V* and put it all together!

$$\iiint_{CV} \frac{\partial U}{\partial t} dV + \iiint_{CV} \nabla \cdot \vec{F}\, dV = \iiint_{CV} S\, dV$$

$$\frac{d}{dt}\frac{1}{V}\iiint_{CV} U dV + \frac{1}{V}\oiint_{\partial CV} (\vec{F} \cdot \hat{n}) dA = \frac{1}{V}\iiint_{CV} S dV$$

$$\frac{d\overline{U}}{dt} + \frac{1}{V}\oiint_{\partial CV} (\vec{F} \cdot \hat{n}) dA = \bar{S}$$

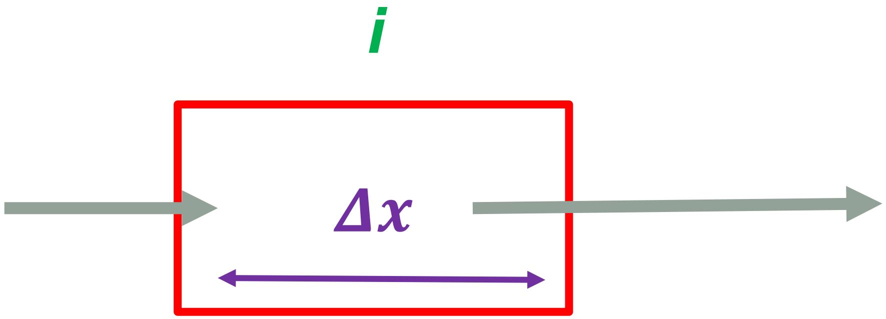
FV General Derivation

$$\frac{d\overline{U}}{dt} = -\frac{1}{V}\oiint_{\partial CV} (\vec{F}\cdot\hat{n})\,dA + \overline{S}$$

- Change in the control volume average $\overline{U}$ is due to stuff leaving and entering control volume, and stuff $\overline{S}$ being created or destroyed on the inside

FV (1D Advection)

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

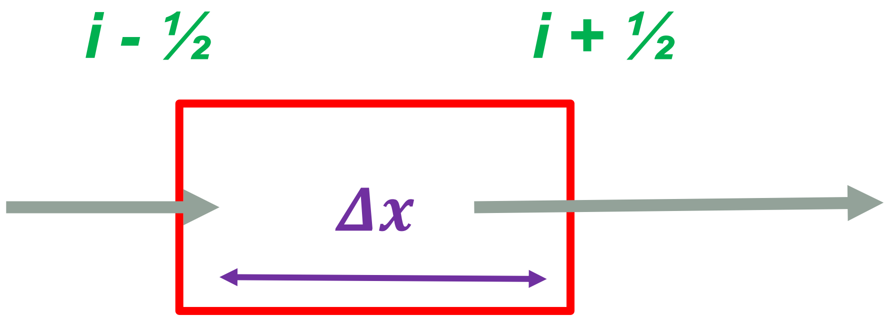


FV (1D Advection)

1) Integrate over control volume CV = CV_i

$$\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} \frac{\partial T}{\partial t} dx + u \int_{i-\frac{1}{2}}^{i+\frac{1}{2}} \frac{\partial T}{\partial x} dx = 0$$

FV (1D Advection)



$$\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} \frac{\partial T}{\partial t} dx + u\left(T_{i+\frac{1}{2}} - T_{i-\frac{1}{2}}\right) = 0$$

FV (1D Advection)

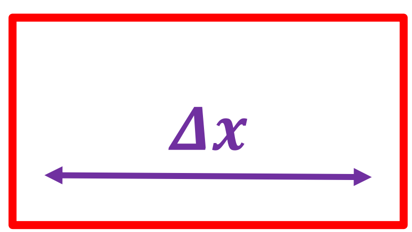
2) Assume CV is fixed (mesh doesn't change)

$$\frac{d}{dt}\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} T\,dx + u\left(T_{i+\frac{1}{2}} - T_{i-\frac{1}{2}}\right) = 0$$

FV (1D Advection)

3) Define CV average

$$\bar{T}_i = \frac{1}{\Delta x}\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} T\,dx$$



FV (1D Advection)

4) Divide through by Δx and put it all together!

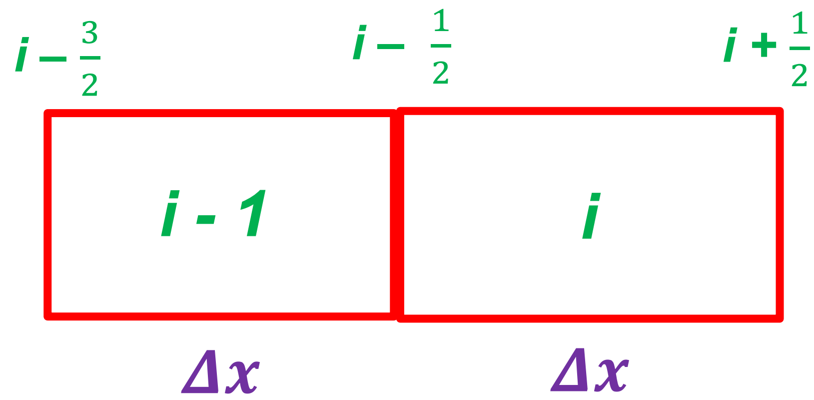
$$\frac{d}{dt}\frac{1}{\Delta x}\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} T dx + \frac{u}{\Delta x}\left(T_{i+\frac{1}{2}} - T_{i-\frac{1}{2}}\right) = 0$$

$$\frac{d\overline{T}_i}{dt} + \frac{u}{\Delta x}\left(T_{i+\frac{1}{2}} - T_{i-\frac{1}{2}}\right) = 0$$

$$\frac{d\overline{U}}{dt} + \frac{1}{V}\oiint_{\partial CV}(\vec{F}\cdot\hat{n})dA = 0$$

FV (1D Advection)

$$T_{i+\frac{1}{2}} = ???, T_{i-\frac{1}{2}} = ???$$



Δx/2

$$\overline{T_i} = \frac{1}{\Delta x}\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} T dx = \frac{1}{\Delta x}\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} \left[T_{i+\frac{1}{2}} + \left.\frac{dT}{dx}\right|_{i+\frac{1}{2}} (x - x_{i+\frac{1}{2}}) + \cdots \right] dx$$

$$\overline{T_{i-1}} = \frac{1}{\Delta x}\int_{i-\frac{3}{2}}^{i-\frac{1}{2}} T dx = \frac{1}{\Delta x}\int_{i-\frac{3}{2}}^{i-\frac{1}{2}} \left[T_{i-\frac{1}{2}} + \left.\frac{dT}{dx}\right|_{i-\frac{1}{2}} (x - x_{i-\frac{1}{2}}) + \cdots \right] dx$$

FV (1D Advection)

$$\overline{T_i} = T_{i+\frac{1}{2}} + \frac{\Delta x}{2}\frac{dT}{\mathrm{d}x}\bigg|_{i+\frac{1}{2}} + \cdots$$

$$\overline{T_{i-1}} = T_{i-\frac{1}{2}} + \frac{\Delta x}{2}\frac{dT}{dx}\bigg|_{i-\frac{1}{2}} + \ \ldots$$

$$\boxed{\frac{d\overline{T_i}}{dt} + \frac{u}{\Delta x}\left(T_{i+\frac{1}{2}} - T_{i-\frac{1}{2}}\right) = 0}$$

$$T_{i+\frac{1}{2}} - T_{i-\frac{1}{2}} = \overline{T_i} + \frac{\Delta x}{2}\frac{dT}{\mathrm{d}x}\bigg|_{i+\frac{1}{2}} - \overline{T_{i-1}} + \frac{\Delta x}{2}\frac{dT}{dx}\bigg|_{i-\frac{1}{2}} + \cdots$$

$$\boxed{T_{i+\frac{1}{2}} - T_{i-\frac{1}{2}} = \overline{T_i} - \overline{T_{i-1}} + \mathcal{O}(\Delta x)}$$

FV (1D Advection)

$$\frac{d\overline{T_i}}{dt} + \frac{u}{\Delta x}\left(T_{i+\frac{1}{2}} - T_{i-\frac{1}{2}}\right) = 0$$

$$T_{i+\frac{1}{2}} - T_{i-\frac{1}{2}} = \overline{T_i} - \overline{T_{i-1}} + \mathcal{O}(\Delta x)$$

$$\frac{d\overline{T_i}}{dt} + u\frac{\left(\overline{T_i} - \overline{T_{i-1}}\right)}{\Delta x} = 0$$

FV Upwind

- 1st order time, space (explicit)

$$\overline{T_i^{n+1}} = \overline{T_i^n} + \Delta t \left(u \frac{\overline{T_i^n} - \overline{T_{i-1}^n}}{\Delta x} \right)$$

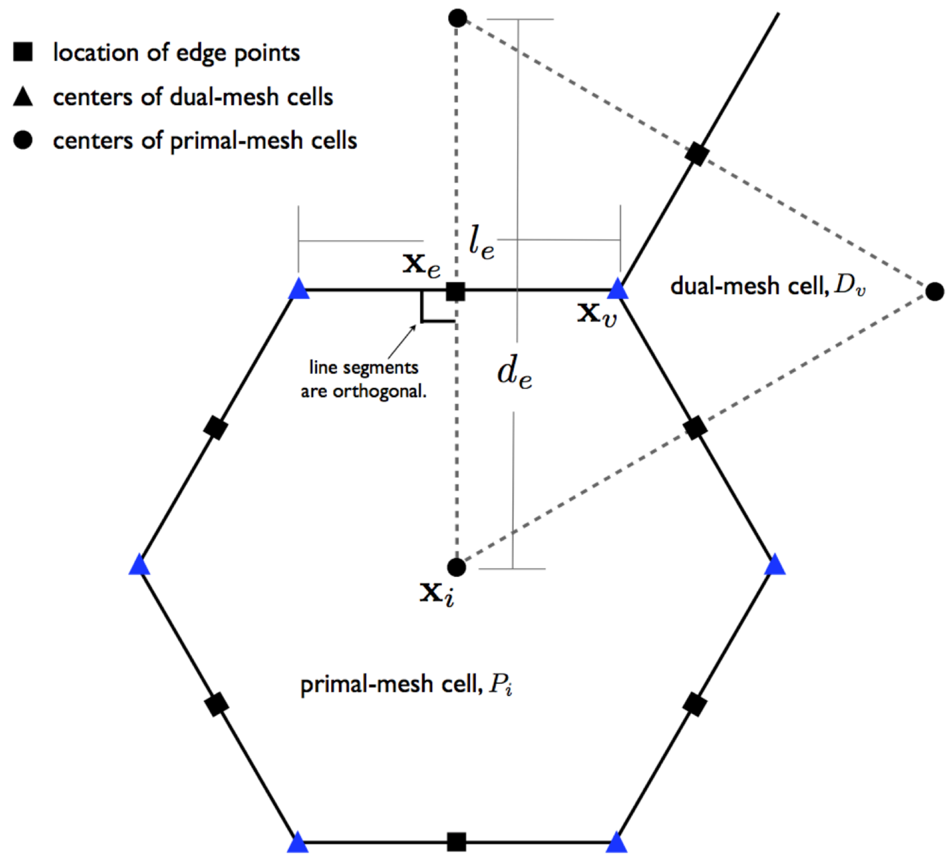
- FD

$$T_i^{n+1} = T_i^n + \Delta t \left(u \frac{T_i^n - T_{i-1}^n}{\Delta x} \right)$$

Summary

- FD operates on points; FV operates on control volumes
  - “Operates” = do Taylor expansions
- FV great for conservation, handling shocks, and weird meshes
- FV used in the MPAS model for its dynamical core

On the final (?) episode of DBZ….



http://www2.mmm.ucar.edu/projects/mpas/mpas_atmosphere_users_guide_6.0.pdf

References

- Arakawa, A., 1966: Computational design for long-term numerical integration of the equations of fluid motion: Two-dimensional incompressible flow. *J. Comput. Phys.*, 1, 119–143.
- Ringler, T. D., D. Jacobsen, M. Gunzburger, L. Ju, M. Duda, and W. Skamarock, 2011: Exploring a Multiresolution Modeling Approach within the Shallow-Water Equations. *Monthly Weather Review.*

Appendix…flux-form equations

$$\frac{\partial \mu v}{\partial y} \approx \frac{(\mu v)_i - (\mu v)_{i-1}}{\Delta y}$$

- Flux-form (conservative)
- If you add up all derivatives for every point, they all cancel except for points at boundaries

Appendix…flux-form equations

$$v\frac{\partial \mu}{\partial y} + \mu\frac{\partial v}{\partial y} \approx v_i\frac{\mu_i - \mu_{i-1}}{\Delta y} + \mu_i\frac{v_i - v_{i-1}}{\Delta y}$$

- Advective-form (non-conservative)
- If you add up all derivatives for every point, no points cancel!
- Location of v_i in $\boldsymbol{v_i}\frac{\mu_i - \mu_{i-1}}{\Delta y}$ is arbitrary