# MPAS NUMERICS, DYNAMICS, AND RESEARCH

Timothy Chui Mar. 21, 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, Dynamic, and Research



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

### Seminar 1: WRF vs. MPAS





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

horizontal grid

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

#### Seminar 1: WRF vs. MPAS



#### WRF Lat-Lon global grid

- Anisotropic grid cells
- Polar filtering required
- Poor scaling on massively parallel computers



MPAS Unstructured Voronoi (hexagonal) grid

- Good scaling on massively parallel computers
- No pole problems

#### Seminar 1: MPAS Forecasts

#### Sea Level Pressure and 100.0-50.0 kPa Thickness

Initialized: 2019-02-14\_00:00:00 Valid: 2019-02-15\_02:00:00 Model/IC: MPAS V6.1/GFS 0.25° 150-30 km variable-resolution grid



Contour Lines: Sea Level Pressure (kPa)

#### Seminar 2: Spherical Centroidal Voronoi Tessellations





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

## Seminar 2: Spherical Centroidal Voronoi Tessellations



• Points associated with a Voronoi region  $V_i$  make up a Voronoi set  $\hat{V}_i$ 

$$\widehat{V}_i = \{ \boldsymbol{x} \in \Omega \mid |\boldsymbol{x} - \boldsymbol{z_i}| < |\boldsymbol{x} - \boldsymbol{z_j}| \text{ for } j = 1, \dots, k, j \neq i \}$$

# Seminar 2: Spherical Centroidal Voronoi Tessellations



In general, the generating point  $z_i$  of each Voronoi region is not the same as the mass centroid  $z_i^*$  of the region

 $z_i \neq z_i^*, i = 1, ..., k$   $z_i = z_i^*, i = 1, ..., k$ 

#### **Seminar 3: Finite-Volume Discretization**

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

• 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



# Table of Contents

- Vertical Coordinate System
- Horizontal Coordinate System
- MPAS Dynamical Equations
- Vertical Discretization
- Horizontal Discretization
- Summary



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

#### **Vertical Coordinate System**



WRF Pressure-based terrain-following sigma vertical coordinate



terrain-following vertical coordinate

• Improved numerical accuracy

http://www2.mmm.ucar.edu/projects/mpas/tutorial/UK2015/slides/MPAS-solver\_physics.pdf

### Vertical Coordinate System

Basic terrain-following (BTF; Gal-Chen and Somerville 1975):

$$z(x, y, \zeta) = \zeta + \left[1 - \frac{\zeta}{z_t}\right] h(x, y)$$

Smoothed terrain-following (STF; Klemp 2011)

$$z(x, y, \zeta) = \zeta + A(\zeta)h_s(x, y, \zeta)$$

 $z(x, y, \zeta) =$  geometric height [m]  $\zeta =$  terrain-following constant; for BTF  $\zeta = z$  at  $z_t$  (model lid) h(x, y) = terrain height [m]  $h_s(x, y, \zeta) =$  terrain influence in STF;  $h_s(x, y, 0) = h$  $A(\zeta) =$  controls how quickly terrain-following -> constant height

# Vertical Coordinate System

#### 15 km grid

#### 7.5 km grid



#### Smoothed hybrid terrain-following (STF) coordinate



http://www2.mmm.ucar.edu/projects/mpas/tutorial/UK2015/slides/MPAS-solver\_physics.pdf

# Vertical Coordinate System - Init

#### • Terrain

- 30 arcsec data averaged over grid-cell areas
- Single pass of smoothing using 4th-order Laplacian
- Vertical Coordinate
  - Choice non-smoothed (BTF) or *n*-times smoothed (STF); iterate upwards from  $h_s^n(x, y, 0) = h$

$$\begin{split} \beta(\zeta) &= \text{smoothing} \\ \text{coefficient} \\ d &= \text{grid-cell length scale} \\ z_H &= \text{height where } \zeta = z \\ \nabla_{\zeta}^2 h_s^n &= \text{Laplacian} \end{split} \qquad \begin{aligned} h_s^{n+1} &= h_s^n + \beta(\zeta) d^2 \nabla_{\zeta}^2 h_s^n \\ A(\zeta) &= \cos^6 \left(\frac{\pi}{2} \frac{\zeta}{z_H}\right), \qquad \zeta < z_H \\ \zeta &\geq z_H \end{aligned}$$

#### Horizontal Coordinate System



#### Horizontal Coordinate System



#### Horizontal Coordinate System



- Geostrophic flow
- Dry
- Incompressible
- Pythagorean

$$u = -\frac{1}{\rho f} \frac{\partial p}{\partial y}$$
$$v = \frac{1}{\rho f} \frac{\partial p}{\partial x}$$

$$a^2 + b^2 = c^2$$

- Coupled variables in conservative form
- Hybrid-height coordinate •
- Nonhydrostatic
- Fully compressible
- Coupled (moist) potential temperature

$$\theta_m = \theta [1 + (R_v/R_d)q_v]$$

$$p = p_0 \left(\frac{R_d \zeta_z \Theta_m}{p_0}\right)^{\gamma}$$

$$\frac{\rho_m}{\rho_d} = 1 + q_v + q_c + q_r + \cdots$$

Skamarock et al. (2012)

$$\begin{split} \frac{\partial \mathbf{V}_{H}}{\partial t} &= -\frac{\rho_{d}}{\rho_{m}} \bigg[ \mathbf{\nabla}_{\zeta} \bigg( \frac{p}{\zeta_{z}} \bigg) - \frac{\partial \mathbf{z}_{H} p}{\partial \zeta} \bigg] - \eta \mathbf{k} \times \mathbf{V}_{H} \\ &- \mathbf{v}_{H} \mathbf{\nabla}_{\zeta} \cdot \mathbf{V} - \frac{\partial \Omega \mathbf{v}_{H}}{\partial \zeta} - \rho_{d} \mathbf{\nabla}_{\zeta} K \\ &- eW \cos \alpha_{r} - \frac{\mathbf{v}_{H} W}{r_{e}} + \mathbf{F}_{\mathbf{V}_{H}}, \\ \frac{\partial W}{\partial t} &= -\frac{\rho_{d}}{\rho_{m}} \bigg[ \frac{\partial p}{\partial \zeta} + g \tilde{\rho}_{m} \bigg] - (\mathbf{\nabla} \cdot \mathbf{v} W)_{\zeta} + \frac{uU + vV}{r_{e}} \end{split}$$

$$\frac{\partial v}{\partial t} = -\frac{\rho_d}{\rho_m} \left[ \frac{\partial p}{\partial \zeta} + g \tilde{\rho}_m \right] - (\nabla \cdot \boldsymbol{v} W)_{\zeta} + \frac{u \sigma + v v}{r_e} + e(U \cos \alpha_r - V \sin \alpha_r) + F_W,$$

$$\frac{\partial \Theta_m}{\partial t} = -(\nabla \cdot \nabla \theta_m)_{\zeta} + F_{\Theta_m},$$

$$\frac{\partial \tilde{\rho}_d}{\partial t} = -(\mathbf{\nabla} \cdot \mathbf{V})_{\zeta}, \quad \text{and}$$

$$\frac{\partial Q_j}{\partial t} = -(\mathbf{\nabla} \cdot \mathbf{V} q_j)_{\zeta} + F_{Q_j}.$$

19

 $\partial$ 

- Coupled variables in conservative form
- Hybrid-height coordinate
- Nonhydrostatic
- Fully compressible
- Coupled (moist) potential temperature

Moist (virtual)  $\theta$ 

$$\begin{aligned} \theta_m &= \theta [1 + (R_v/R_d)q_v] \\ p &= p_0 \Big( \frac{R_d \zeta_z \Theta_m}{p_0} \Big)^{\gamma} \quad \text{Eqn of state} \\ \frac{\rho_m}{\rho_d} &= 1 + q_v + q_c + q_r + \cdots \\ \text{Skamarock et al. (2012)} & \text{Moist air} \end{aligned}$$

$$\frac{\mathbf{V}_{H}}{\partial t} = -\frac{\rho_{d}}{\rho_{m}} \left[ \mathbf{\nabla}_{\zeta} \left( \frac{p}{\zeta_{z}} \right) - \frac{\partial \mathbf{z}_{H} p}{\partial \zeta} \right] - \eta \mathbf{k} \times \mathbf{V}_{H} 
- \boldsymbol{v}_{H} \mathbf{\nabla}_{\zeta} \cdot \mathbf{V} - \frac{\partial \Omega \boldsymbol{v}_{H}}{\partial \zeta} - \rho_{d} \mathbf{\nabla}_{\zeta} K 
- eW \cos \alpha_{r} - \frac{\boldsymbol{v}_{H} W}{r_{e}} + \mathbf{F}_{\mathbf{V}_{H}},$$

$$\frac{\partial W}{\partial t} = -\frac{\rho_d}{\rho_m} \left[ \frac{\partial p}{\partial \zeta} + g \tilde{\rho}_m \right] - (\nabla \cdot \boldsymbol{v} W)_{\zeta} + \frac{u U + v V}{r_e} + e(U \cos \alpha_r - V \sin \alpha_r) + F_W,$$

$$\frac{\partial \Theta_m}{\partial t} = -(\nabla \cdot \nabla \theta_m)_{\zeta} + F_{\Theta_m},$$
  
Temperature  
$$\frac{\partial \tilde{\rho}_d}{\partial t} = -(\nabla \cdot \nabla)_{\zeta}, \text{ and } \text{Continuity}$$

 $\frac{\partial Q_j}{\partial t} = -(\mathbf{\nabla} \cdot \mathbf{V} q_j)_{\zeta} + F_{Q_j}.$ 

Moisture

Flux-form prognostic equations

$$(U, V, W, \Theta_m, Q_j) = \widetilde{\rho_d} \cdot (u, v, w, \theta_m, q_j)$$

j = v (vapour), c (cloud), r (rainwater), etc.

$$\widetilde{\rho_d} = \rho_d \left( \frac{1}{\frac{d\zeta}{dz}} \right) = \rho_d \zeta_z$$

$$\boldsymbol{v} = (u, v, w), \boldsymbol{V} = (U, V, W)$$

Vertical momentum

$$\begin{aligned} \frac{\partial W}{\partial t} &= -\frac{\rho_d}{\rho_m} \left[ \frac{\partial p}{\partial \zeta} + g \tilde{\rho}_m \right] - \left( \nabla \cdot \boldsymbol{v} W \right)_{\zeta} + \frac{u U + v V}{r_e} \\ &+ e(U \cos \alpha_r - V \sin \alpha_r) + F_W, \end{aligned}$$

Vertical momentum



Horizontal momentum



#### Horizontal momentum



### **Transport (Advection)**

•  $\psi$  = some quantity

$$\frac{\partial \rho \psi}{\partial t} = -\nabla_{\zeta} \cdot \mathbf{v}_{\mathbf{H}}(\rho \psi) - \frac{\partial W \rho \psi}{\partial z}$$

# Scalar Transport

• FV formulation over, integrate over cell

$$\int_{V} \frac{\partial \rho \psi}{\partial t} dV = -\int_{V} \left( \nabla \cdot \mathbf{v}(\rho \psi) \right) dV$$

### Scalar Transport

- Apply divergence theorem; controlvolume average definition
- $\Sigma$  = surface of polyhedron;  $d\sigma$  = surface element

$$\frac{\partial \overline{\rho \psi}}{\partial t} = -\frac{1}{V} \int_{\Sigma} (\rho \psi) \mathbf{v} \cdot \mathbf{n} d\sigma$$

7	Vertical Discretization $W = \rho W$		
∠ ↑		k+2 -	stencil $\delta_z^2 \psi_k = \psi_{k-1} - 2\psi_k + \psi_{k+1}$
	$F(W,\psi)_{k+\frac{1}{2}}$	k+1/2 k+1/2 k k-1/2 k-1 -	$F(W, \psi)_{k+\frac{1}{2}} = W_{k+\frac{1}{2}} \left[ \frac{1}{2} (\psi_{k+1} + \psi_k) - \frac{1}{12} (\delta_z^2 \psi_{k+1} + \delta_z^2 \psi_k) + sign(W) \frac{\beta}{12} (\delta_z^2 \psi_{k+1} - \delta_z^2 \psi_k) \right]$
		k-2	eta = 0: 4 <sup>th</sup> -order scheme, neutral $eta > 0$ : 3 <sup>rd</sup> -order scheme, damping

 Sum counter-clockwise around hexagon edges



https://www.earthsystemcog.org/site\_media/projects/dycore\_test\_group/20160122\_M PAS\_configuration\_overview.pdf



$$F(U,\psi)_{i+\frac{1}{2}}$$
  
=  $U_{i+\frac{1}{2}} \Big[ \frac{1}{2} (\psi_{i+1} + \psi_i) - \frac{1}{12} (\delta_x^2 \psi_{i+1} + \delta_x^2 \psi_i) + sign(U) \frac{\beta}{12} (\delta_x^2 \psi_{i+1} - \delta_x^2 \psi_i) \Big]$ 

- *x* = direction normal to cell edges
- Coordinates aren't next to each other in the horizontal; can't do straight-forward computation of  $\delta_x^2 \psi_i$

$$\delta_x^2 \psi_i = \Delta x^2 \frac{\partial^2 \psi}{\partial x^2} + \mathcal{O}(\Delta x^4)$$

$$\begin{split} F(U,\psi)_{i+\frac{1}{2}} &= U_{i+\frac{1}{2}} \left[ \frac{1}{2} (\psi_{i+1} + \psi_i) \\ &- \Delta x_e^2 \frac{1}{12} \left\{ \left( \frac{\partial^2 \psi}{\partial x^2} \right)_{i+1} + \left( \frac{\partial^2 \psi}{\partial x^2} \right)_i \right\} \\ &+ sign(U) \Delta x_e^2 \frac{\beta}{12} \left\{ \left( \frac{\partial^2 \psi}{\partial x^2} \right)_{i+1} - \left( \frac{\partial^2 \psi}{\partial x^2} \right)_i \right\} \end{split}$$

https://www.earthsystemcog.org/site\_media/proje cts/dycore\_test\_group/20160122\_MPAS\_configur ation\_overview.pdf

$$F(U,\psi)_{i+\frac{1}{2}}$$

$$= U_{i+\frac{1}{2}} \left[ \frac{1}{2} (\psi_{i+1} + \psi_i) - \Delta x_e^2 \frac{1}{12} \left\{ \left( \frac{\partial^2 \psi}{\partial x^2} \right)_{i+1} + \left( \frac{\partial^2 \psi}{\partial x^2} \right)_i \right\} + sign(U) \Delta x_e^2 \frac{\beta}{12} \left\{ \left( \frac{\partial^2 \psi}{\partial x^2} \right)_{i+1} - \left( \frac{\partial^2 \psi}{\partial x^2} \right)_i \right\} \right]$$

$$\psi_{3}$$

$$\psi_{2}$$

$$\psi_{1}$$

$$\psi_{3}$$

$$\psi_{0}$$

$$\psi_{1}$$

$$\psi_{7}$$

$$\psi_{4}$$

$$\psi_{6}$$

$$\psi_{5}$$

#### Fit polynomial to approximate second derivatives (Skamarock and Gassmann 2011)

https://www.earthsystemcog.org/site\_media/proje cts/dycore\_test\_group/20160122\_MPAS\_configur ation\_overview.pdf



#### Fit polynomial to approximate second derivatives (Skamarock and Gassmann 2011)

# Not discussed



https://www.convertwithcontent.com/webmarketing-in-a-nutshell/

- Derivations
- Types of hybrid coordinates
- Nonlinear Coriolis term
- Kinetic energy gradient
- Explicit spatial filters
- Time discretization (split-explicit RK3); treatment of acoustic modes
- Top-of-model Rayleigh damping

# Summary

- MPAS is a cool model
- Hybrid-height, terrain-influenced vertical coordinate
- C-Grid staggering on a Voronoi mesh
- Nonhydrostatic, conservative equations
- Sophisticated FV discretization on an unstructured mesh



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

### Thank you (???)



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

#### 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.
- Gal-Chen, T., and R.C.J. Somerville, 1975: On the use of a coordinate transformation for the solution of the Navier-Stokes equations. J. Comput. Phys., 17, 209-228, doi:10.1016/0021-9991(75)90037-6.Klemp, J. B., 2011: A Terrain-Following Coordinate with Smoothed Coordinate Surfaces. *MWR*, 139, 2163-2169, doi: 10.1175/MWR-D-10-05046.1.
- 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. *MWR*, **139**, doi: 10.1175/MWR-D-10-05049.1.
- Skamarock, W. C., J. B. Klemp, J. Dudhia, D. O. Gill, D. M. Barker, W. Wang and J. G. Powers, 2008: A description of the Advanced Research WRF version 3. NCAR Technical note -475+STR
- Skamarock, W. C., and A. Gassmann, 2011: Conservative Transport Schemes for Spherical Geodesic Grids: High-Order Flux Operators for ODE-Based Time Integration. *MWR*, **139**, 2962-2975, doi: 10.1175/MWR-D-10-05056.1.
- Skamarock, W. C., J. B. Klemp, M. Duda, L. D. Fowler, and S. H. Park, 2012: A multiscale nonhydrostatic atmospheric model using centroidal Voronoi tesselations and C-grid staggering. *MWR*, 140, 3090 – 3105, doi: 10.1175/MWR-D-11-00215.1.