

### The Model for Prediction Across Scales Atmosphere

### MPAS-Atmosphere and the future



MPAS-A and GPUs

NVIDIA Ampere A100 GPU

MPAS virtual tutorial, 1-3 May 2023

MPAS-A in an Earth System Model



Deep-Atmosphere MPAS-A





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Bill Skamarock, NCAR/MMM, for the MMM-MPAS team and many community collaborators





## Coming in the next release (Version 8):

- Physics updates
- Clean-up in dynamics parallelization
- Support for the use of MPAS-A dynamics in CESM
- New I/O library (SMIOL); alternative to PIO
- New halo exchange infrastructure (support GPUs)
- Updates to LBCs in regional MPAS to improve robustness
- Additional post-processing capabilities



# MPAS and GPUs



NVIDIA Ampere A100 GPU

We released the GPU-enabled MPAS-Atmosphere in October 2020 as a branch from MPAS Version 6.1. We have a Version 7 update but it has not been released.

What is in current (2020) release:

- GPU-enabled MPAS dynamical core using OpenACC directives.
- Some GPU-enabled physics (e.g. YSU, WSM6, M-O, scale-aware nTiedtke)
- Asynchronous execution capability on heterogenous architectures currently radiation (lagged) and NOAH land model on CPUs, all else on GPUs
- Configurations tested and validated on IBM POWER9 architectures and on AMD architectures employing NVIDIA V100 and A100 GPUs.



# MPAS and GPUs

We released the GPU-enabled MPAS-Atmosphere in October 2020 as a branch from MPAS Version 6.1. We have a Version 7 update but it has not been released.

NVIDIA Ampere A100 GPU

What is *NOT* in this release:

- Regional capability
- Most of the physics options

Extending the global GPU capability to regional is straightforward. Additional physics ports to GPUs take significant time and resources; we are leveraging other projects to enable additional GPU physics.



# MPAS and GPUs – Plans

NCAR's next supercomputer will have significant GPU capabilities. DERECHO – 82 GPU nodes (4 A100 GPUs per node).



As DERECHO becomes available

- Test and release global configurations
- Enable regional configurations, test and release
- Bring in other GPU-capable physics as they become available
  - RRTMG-P
  - Other microphysics (MG3/PUMAS)
- MPAS single-source release of the of the dynamical core, separate GPU and CPU physics

Issue: Moving (physics community) developers to GPU code.





# System for Integrated Modeling of the Atmosphere (SIMA)

SIMA is composed of common atmospheric model components & infrastructure embedded in an earth-system model

#### **SIMA Vision**

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- Encompass Climate, Weather, Chemistry & Geospace
- Prediction (Initialized and Forecast) capabilities
- Complement & extend existing applications (CESM/WRF/MPAS)
- Shared infrastructure for efficiency
- Minimal set of components
- 'Center Wide' project including education, observations, computation





# System for Integrated Modeling of the Atmosphere (SIMA)

(1) MPAS-Atmosphere in an Earth System
Model (ESM), using CESM components.
Other ESM components: ocean, land,
land and sea ice, chemistry

(2) WRF/MPAS physics in an ESM using the Common Community Physics Package (CCPP) interface.

#### <u>Status:</u>

- MPAS-A in CESM is being tested.
- Only CESM/CAM physics will be available in this first release.
- CCPP implementation in MPAS and CESM is not yet complete.
- Initial release (experimental) TBD.





 $\Delta \mathbf{x} = \Delta \mathbf{x}_0 \ \mathbf{r/r}_e$ 

## Deep Atmosphere: Geometry

$$\frac{\partial \tilde{\rho}}{\partial t} = \nabla_{\zeta} \cdot \mathbf{V}_{\mathbf{H}} + \frac{\partial \Omega}{\partial \zeta} \qquad \tilde{\rho} = \frac{\rho}{\zeta_{z}}, \quad \mathbf{V}_{\mathbf{H}} = (U, V) = (\tilde{\rho}u, \tilde{\rho}v), \quad \Omega = \tilde{\rho}\dot{\zeta} \quad \text{(shallow atmosphere)}$$

$$\frac{\partial \tilde{\rho}}{\partial t} = \frac{1}{A_{0}} \sum_{i=1}^{n} U_{i}l_{0_{i}} + \frac{\Delta \Omega}{\Delta \zeta} \qquad \text{horizontal} \quad \mathbf{vertical}$$

$$\frac{\partial \tilde{\rho}}{\partial t} = \frac{1}{A_{0}} \sum_{i=1}^{n} U_{i}l_{0_{i}} + \frac{\Delta \Omega}{\Delta \zeta} \qquad A_{0}, l_{0_{i}} = \text{ Cell area and edge lengths at surface}$$
Shallow Atmosphere:  $\tilde{\rho} = \frac{\rho}{\zeta_{z}}, \quad U_{i} = \tilde{\rho}u_{i}, \qquad \Omega = \tilde{\rho}\dot{\zeta} \quad (A = A_{0}, \quad l_{i} = l_{0_{i}})$ 
Deep Atmosphere:  $\tilde{\rho} = \frac{A}{A_{0}}\frac{\rho}{\zeta_{z}}, \quad U_{i} = \frac{A_{0}}{A}\frac{l_{i}}{l_{0_{i}}}\tilde{\rho}u_{i}, \quad \Omega = \tilde{\rho}\dot{\zeta}$ 

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Shallow atmosphere



 $\frac{\partial U}{\partial t} = -\frac{\rho_d}{\rho_m} \left| \nabla_{\zeta} \left( \frac{p}{\zeta_z} \right) + \rho_m g \, \nabla_{\zeta} z \right| - \eta \, \mathbf{k} \times \mathbf{V}_H$  $-\mathbf{v}_{H}\nabla_{\zeta}\cdot\mathbf{V}-\frac{\partial\Omega\mathbf{v}_{H}}{\partial\zeta}-\tilde{\rho}_{d}\nabla_{\zeta}K+\mathbf{F}_{V_{H}}$  $\frac{\partial W}{\partial t} = -\frac{\rho_d}{\rho_m} \left[ \frac{\partial p}{\partial \zeta} + g \tilde{\rho}_m \right] - \left( \nabla \cdot \mathbf{v} \, W \right)_{\zeta} + F_W$ 
$$\begin{split} \frac{\partial U}{\partial t} &= -\frac{\rho_d}{\rho_m} \left[ \nabla_{\zeta} \left( \frac{p}{\zeta_z} \right) + \rho_m g \left( \frac{r_e}{r} \right)^2 \right] \nabla_{\zeta} z \right] - \eta \, \mathbf{k} \times \mathbf{V}_H \\ &- \mathbf{v}_H \nabla_{\zeta} \cdot \mathbf{V} - \frac{\partial \Omega \mathbf{v}_H}{\partial \zeta} - \tilde{\rho}_d \nabla_{\zeta} K + \mathbf{F}_{V_H} \end{split}$$
 $-\left( eW\cos lpha _{r}+rac{uW}{2}
ight)$  $\frac{\partial W}{\partial t} = -\frac{\rho_d}{\rho_m} \left[ \frac{\partial p}{\partial \zeta} + \left( g \left( \frac{r_e}{r} \right)^2 \right) \tilde{\rho}_m \right] - \left( \nabla \cdot \mathbf{v} \, W \right)_{\zeta} + F_W$  $\underbrace{uU+vV}_{}+e\left(U\cos\alpha_{r}-V\sin\alpha_{r}\right)$ 

Deep atmosphere

Additional terms Gravity —— Coriolis ——

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Baroclinic wave test, reduced radius sphere (radius =  $r_e/20$ ,  $\Omega = 20 \Omega_e$ )



(Ullrich et al 2013, JAMES)





Further out:

- Development and release of a geospace capable solver (2D prototype design and testing are largely complete).
  - Variable (prognostic) constituents (O, O<sub>2</sub>, N<sub>2</sub>); doi:10.1029/2021MS002499 (JAMES 2021)
  - Constant pressure upper boundary condition to accommodate thermospheric diurnal heating/cooling; doi:10.1175/MWR-D-21-0328.1 (MWR 2022)
  - Numerics for large physical viscosities
  - Geospace physics





## Also under development...

LES capabilities – we have an LES branch that incorporates a 3D Smagorinsky (diagnostic) scheme and a 1.5 order prognostic TKE scheme.

Scalar transport in physics parameterizations (convection, boundary layer)

Prognostic ozone

Mesh generation, global and regional





Coming Events

Version 8 release - before the WRF-MPAS Workshop this June (2023)

WRF-MPAS workshop Tues-Fri 20-23 June 2023 (in person). Registration opens 15 May

MPAS + MPAS-JEDI tutorial, 18-22 September 2023 (in person)

We've begun work on an MPAS NCAR Technical Note. Available sometime 2024

