NAVAL POSTGRADUATE SCHOOL

The Development of the Non-hydrostatic Unified Model of the Atmosphere (NUMA)

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Background

Currently, in the U.S. there is a movement to construct one NWP model (NWS, Navy, Air Force – other partners include NASA and DOE). This National Board (NUOPC=National Unified Operational Prediction Capability) aims to develop a new model that is:

1. Highly scalable on current and future computer architectures
2. Global model that is valid at the meso-scale (i.e., non-hydrostatic)
3. Applicable to medium-range NWP and decadal time-scales

Motivation

Our goal is to construct numerical methods for non-hydrostatic mesoscale and global atmospheric models (for NWP applications).

To verify our numerical methods we have built a modeling framework with the following capabilities:

1. Highly scalable on current and future computer architectures (exascale computing: this means CPUs and GPUs)
2. Flexibility to use a wide range of grids (e.g., statically and dynamically adaptive)
3. Model that is accurate, robust, and fully conservative

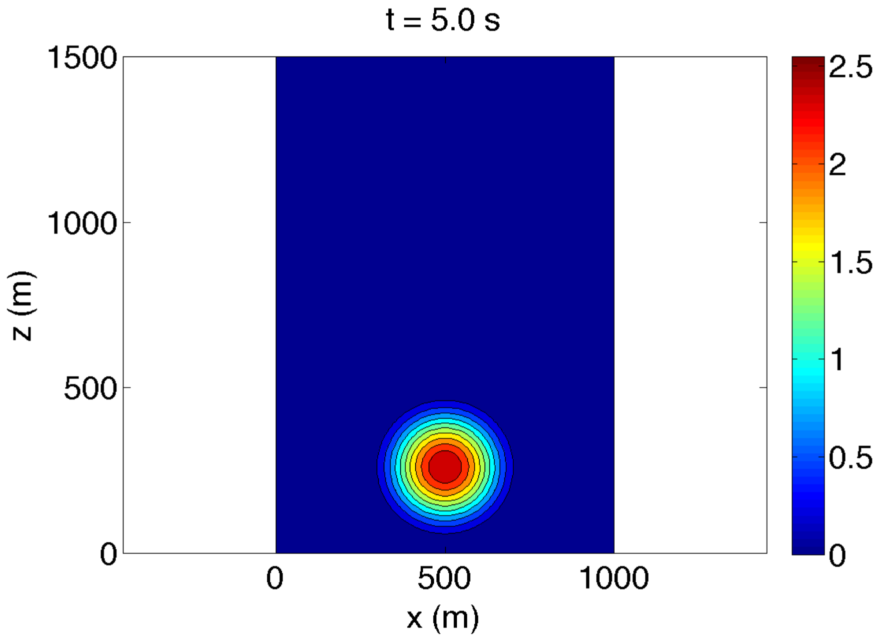
Talk Summary

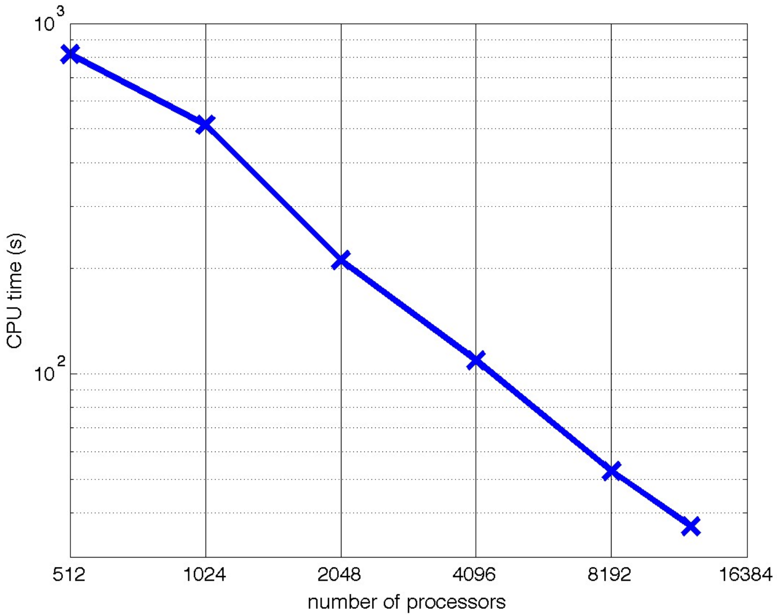
1. New models need to exploit available computers
2. Numerical methods in new GFD models
3. Desired properties of our future GFD models
4. NUMA Model

Talk Summary

1. New models need to exploit available computers
    - Clock-speeds no longer getting faster; vendors are just giving us more CPUs
    - From Terascale to Petascale/Exascale Computing
    - 10 of Top 500 are already in the Petascale range
    - 3 of top 10 are GPU-based machines
2. Numerical methods in new GFD models
3. Desired properties of our future GFD models
4. NUMA Model

Example of Linear (Perfect) Scalability





NUMA-CG Simulation with 16 Million Grid Points

Talk Summary

1. New models need to exploit available computers
2. Numerical methods in new GFD models
   - Time-Integration is important (e.g., explict, fully-implicit, semi-implicit)
   - Spatial Discretization methods is how we are able to take advantage of Parallel computers (i.e., domain decomposition of the physical grid)
3. Desired properties of our future GFD models
4. NUMA Model

Time Integration

- Explicit methods
- Fully-implicit methods
- Implicit-Explicit (IMEX) methods
  - Linear Multi-step Methods
  - Multi-stage Methods
  - Multi-rate Methods

Multi-step/Multi-stage IMEX Methods

- Let's write the governing equations as

$$\frac{d\mathbf{q}}{dt} = S(\mathbf{q})$$

- If we knew the linear operator L (containing the fastest waves in the system), then we could write

$$\frac{d\mathbf{q}}{dt} = \left\{ S(\mathbf{q}) - \delta_{SI} L(\mathbf{q}) \right\} + \delta_{SI} \left[L(\mathbf{q}) \right]$$

- Discretizing by a Kth order time-integrator yields

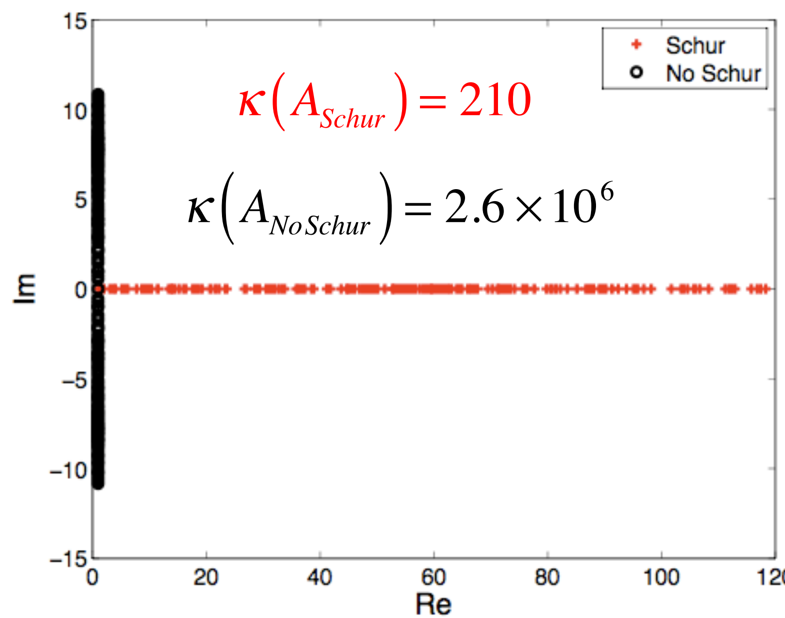
$$\mathbf{q}_{tt} = \hat{\mathbf{q}} + \lambda L\left(\mathbf{q}_{tt}\right) \longrightarrow \left(I - \lambda L\right)\mathbf{q}_{tt} = \hat{\mathbf{q}} \longrightarrow \mathbf{A}\mathbf{x} = \mathbf{b}$$

IMEX Methods
(Important Properties of Schur Complement)

No Schur → **Schur**

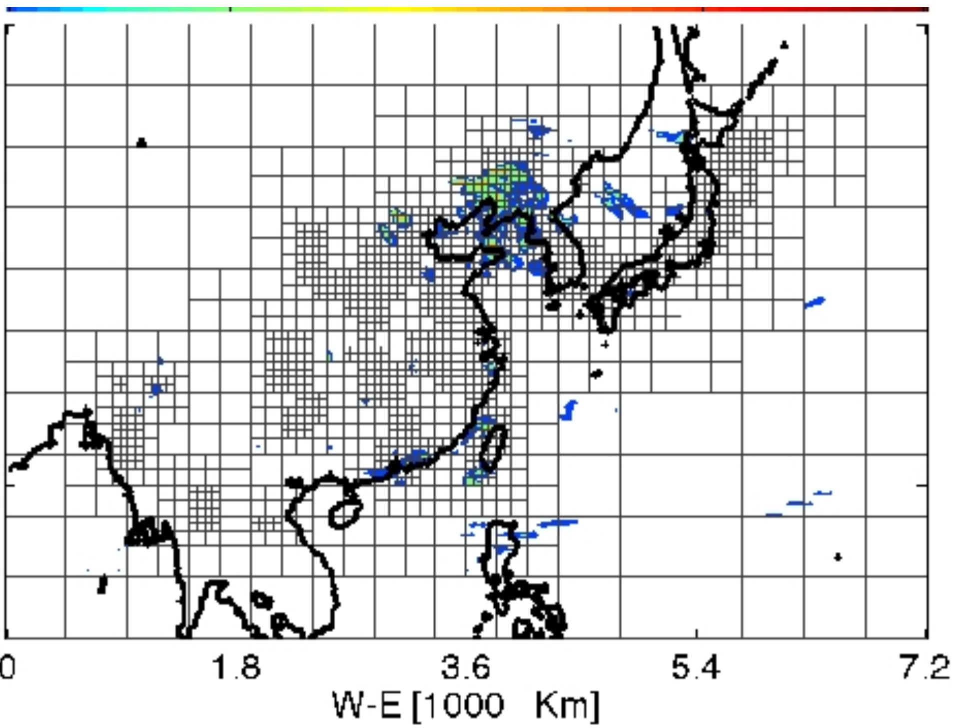
$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{tt} \\ \varphi_{tt} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \longrightarrow \begin{pmatrix} A_{11} & A_{12} \\ 0 & A_{22} - A_{21}A_{11}^{-1}A_{12} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{tt} \\ \varphi_{tt} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 - A_{21}A_{11}^{-1}b_1 \end{pmatrix}$$

- The Schur system is clearly smaller than the original (No Schur) system (NxN instead of 3Nx3N for 2D SWE).
- Equally important is that the Schur System is better conditioned than the original system. This means that fewer iterations are required by an iterative solver to reach convergence.
- **Key Point**: Eigenvalues of the Schur form lie in the region where GMRES will perform well.

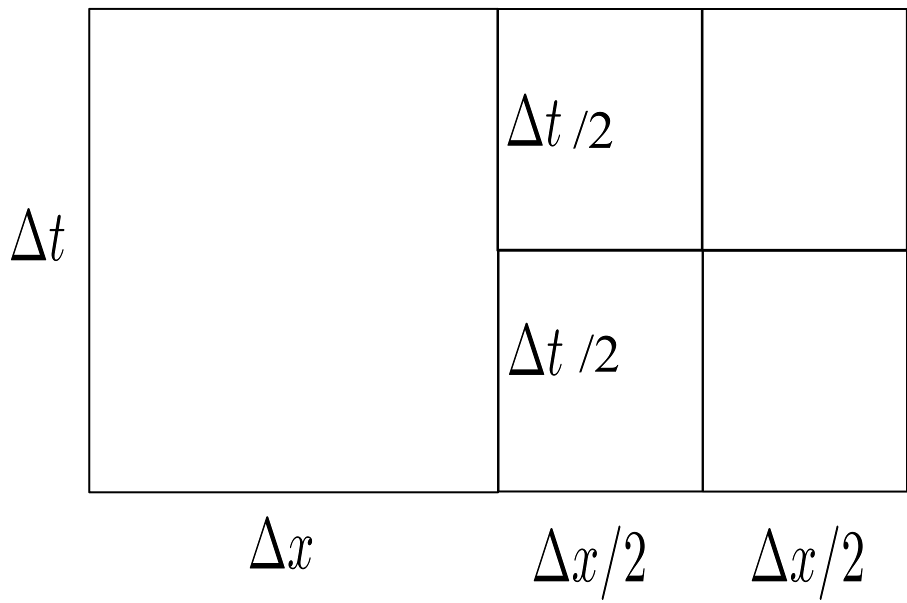


2D Euler Equations

Multi-Rate Methods



Adaptive Mesh Refinement (Space)



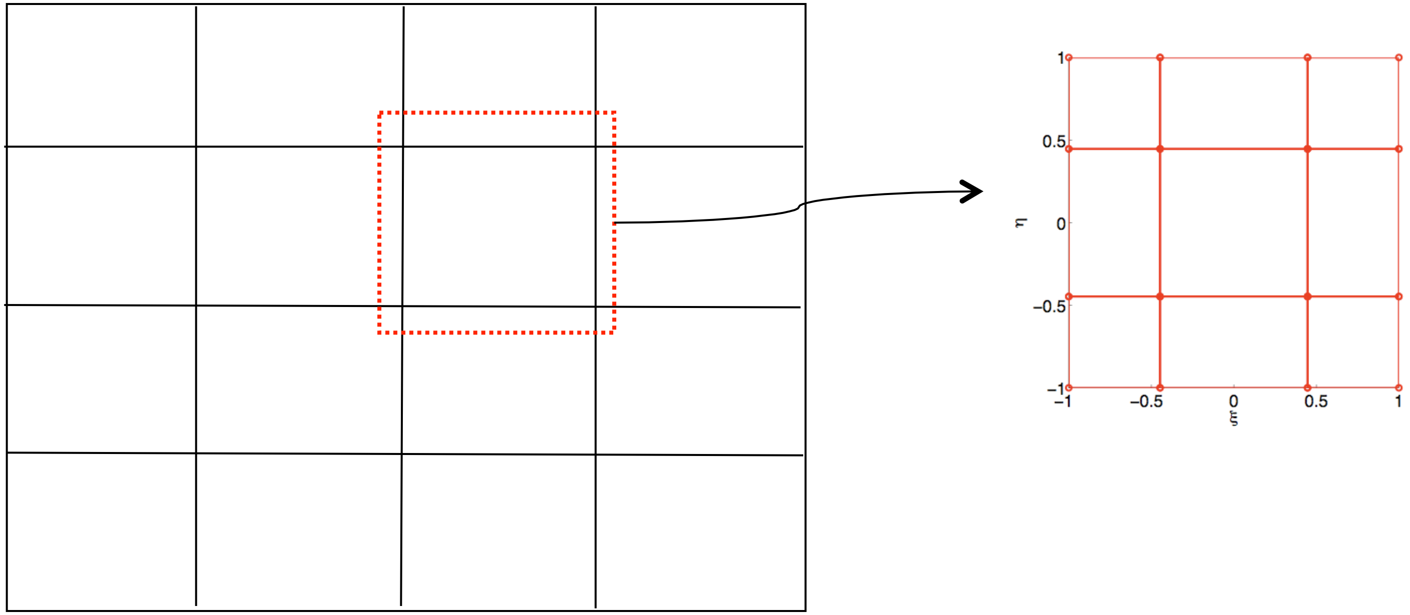
Multi-rate Time-Integration (Space-Time)

Spatial Discretization Methods

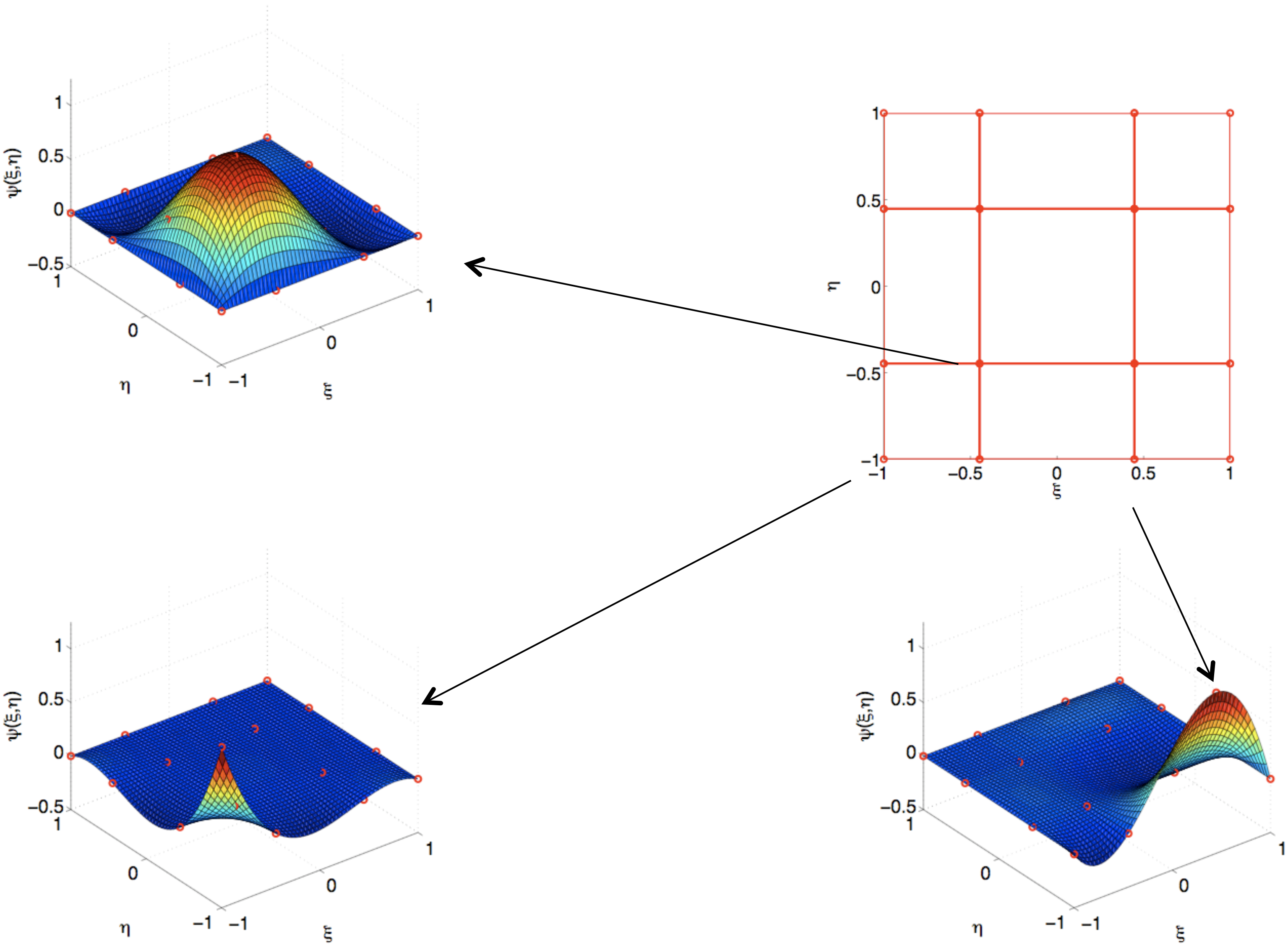
- Element-based Galerkin Methods
  - Continuous Galerkin
  - Discontinuous Galerkin

Element-based Galerkin (EBG) Methods
(Definition and Examples)

- An element is chosen to be the basic building-block of the discretization and then a polynomial expansion is used to represent the solution inside the element



Element-based Galerkin Methods (N=3 Basis Function Expansion)



Spatial Discretization

- Primitive Equations: $$\frac{\partial q}{\partial t} + \nabla \cdot \mathbf{F} = S(q)$$

- Approximate the solution as: $$q_N = \sum_{i=1}^{M_N} \psi_i \, q_i \qquad \mathbf{F}_N = \mathbf{F}\left(q_N\right) \qquad S_N = S\left(q_N\right)$$
  - **Interpolation O(N)**

- Write Primitive Equations as: $$R(q_N) \equiv \frac{\partial q_N}{\partial t} + \nabla \cdot \mathbf{F}_N - S_N = \varepsilon$$

- Weak Problem Statement: Find $q_N \in \Sigma(\Omega) \; \forall \; \psi \in \Sigma$

$$\Sigma = \left\{ \psi \in H^1(\Omega) : \psi \in P_N(\Omega_e) \forall \Omega_e \right\} \qquad \text{(CG)}$$

$$\Sigma = \left\{ \psi \in L^2(\Omega) : \psi \in P_N(\Omega_e) \forall \Omega_e \right\} \qquad \text{(DG)}$$

  - such that (**Integration O(2N)**)

$$\int_{\mathbf{\Omega_e}} \psi R\left(q_N\right) d\Omega_e = 0$$

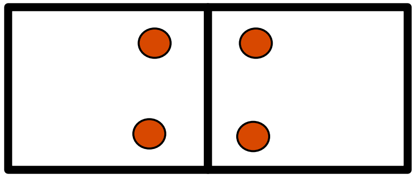
Spatial Discretization

- Integral Form: $$\int_{\Omega_e} \psi R(q_N)\, d\Omega_e = 0$$
- Matrix Form: $$L_i(q) \equiv M_{ij}^{(e)} \frac{dq_j^{(e)}}{dt} - \left(\mathbf{D}_{ij}^{(e)}\right)^T \mathbf{F}_j^{(e)} - S_i^{(e)} = 0$$
- Communicator: $$\mathbf{C}\left(L(q)\right)$$
- Where each matrix is: $$M_{ij}^{(e)} = \int_{\Omega_e} \psi_i \psi_j \, d\Omega_e$$ ← **Integration O(2N)**

$$\mathbf{D}_{ij}^{(e)} = \int_{\Omega_e} \nabla \psi_i \psi_j \, d\Omega_e$$

For DG: $$\mathbf{C}\left(L_i(q)\right) = L_i(q) + \left(\mathbf{M}_{ij}^{\Gamma}\right)^T \mathbf{F}_j^{(*)}$$ → $$\mathbf{M}_{ij}^{\Gamma} = \int_{\Gamma} \mathbf{n} \psi_i \psi_j \, d\Gamma$$

For CG: $$\mathbf{C}\left(L_i(q)\right) = \mathrm{S}\left(\mathrm{G}(q)\right)$$



$q_i^{(e)}$

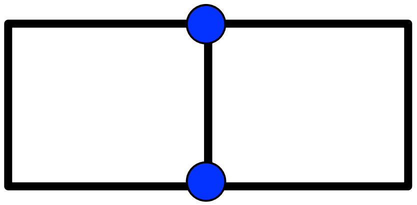
Spatial Discretization

- Integral Form: $$\int_{\Omega_e} \psi R(q_N)\, d\Omega_e = 0$$
- Matrix Form: $$L_i(q) \equiv M_{ij}^{(e)} \frac{dq_j^{(e)}}{dt} - \left(\mathbf{D}_{ij}^{(e)}\right)^T \mathbf{F}_j^{(e)} - S_i^{(e)} = 0$$
- Communicator: $$\mathbf{C}\left(L(q)\right)$$
- Where each matrix is: $$M_{ij}^{(e)} = \int_{\Omega_e} \psi_i \psi_j \, d\Omega_e$$ ← **Integration O(2N)**

$$\mathbf{D}_{ij}^{(e)} = \int_{\Omega_e} \nabla \psi_i \psi_j \, d\Omega_e$$

For DG: $$\mathbf{C}\left(L_i(q)\right) = L_i(q) + \left(\mathbf{M}_{ij}^{\Gamma}\right)^T \mathbf{F}_j^{(*)} \longrightarrow \mathbf{M}_{ij}^{\Gamma} = \int_{\Gamma} \mathbf{n} \psi_i \psi_j \, d\Gamma$$

For CG: $$\mathbf{C}\left(L_i(q)\right) = \mathrm{S}\left(\mathrm{G}(q)\right)$$



$$q_I = \mathrm{G}\left(q_i^{(e)}\right) \quad (i,e) \longrightarrow I$$

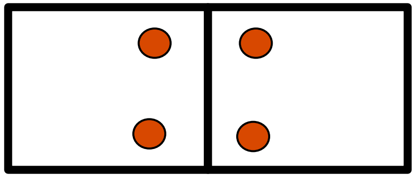
Spatial Discretization

- Integral Form: $$\int_{\Omega_e} \psi R(q_N)\, d\Omega_e = 0$$
- Matrix Form: $$L_i(q) \equiv M_{ij}^{(e)} \frac{dq_j^{(e)}}{dt} - \left(\mathbf{D}_{ij}^{(e)}\right)^T \mathbf{F}_j^{(e)} - S_i^{(e)} = 0$$
- Communicator: $$\mathbf{C}\left(L(q)\right)$$
- Where each matrix is: $$M_{ij}^{(e)} = \int_{\Omega_e} \psi_i \psi_j \, d\Omega_e$$ ← **Integration O(2N)**

$$\mathbf{D}_{ij}^{(e)} = \int_{\Omega_e} \nabla \psi_i \psi_j \, d\Omega_e$$

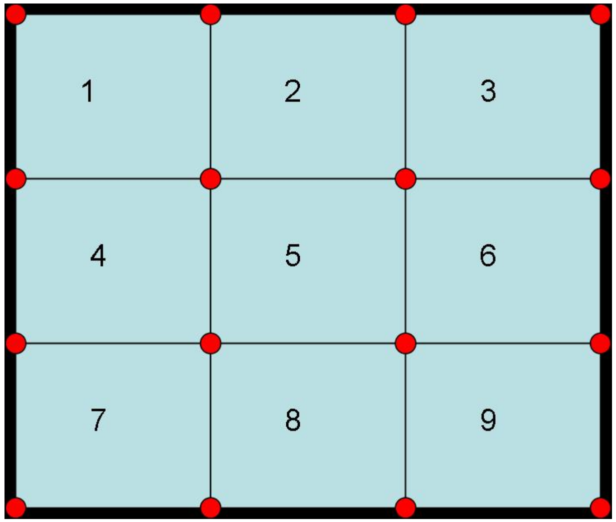
For DG: $$\mathbf{C}\left(L_i(q)\right) = L_i(q) + \left(\mathbf{M}_{ij}^{\Gamma}\right)^T \mathbf{F}_j^{(*)} \longrightarrow \mathbf{M}_{ij}^{\Gamma} = \int_{\Gamma} \mathbf{n} \psi_i \psi_j \, d\Gamma$$

For CG: $$\mathbf{C}\left(L_i(q)\right) = \mathrm{S}\left(\mathrm{G}(q)\right)$$



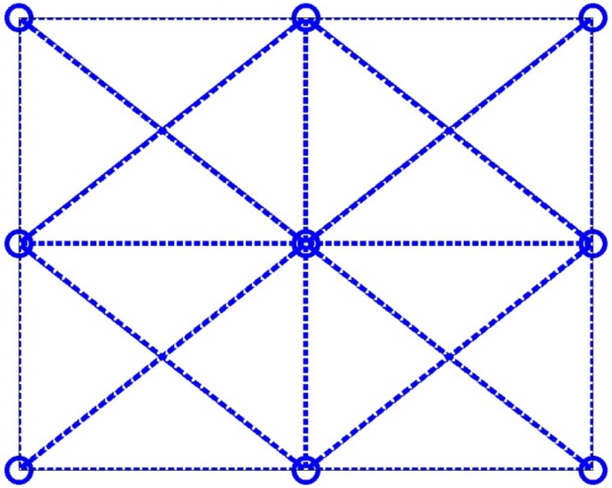
$$q_i^{(e)} = \mathrm{S}\left(q_I\right) \quad I \longrightarrow (i,e)$$

Domain Decomposition: Adjacency Matrices

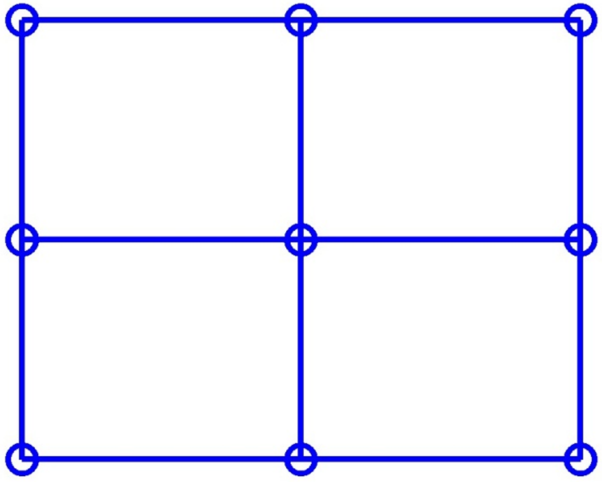


Max number of neighbors

Geometry	**CG**	**DG**
Quadrilaterals	8	4
Hexahedra	26	6
Triangles	ND	3



CG Adjacency



DG Adjacency

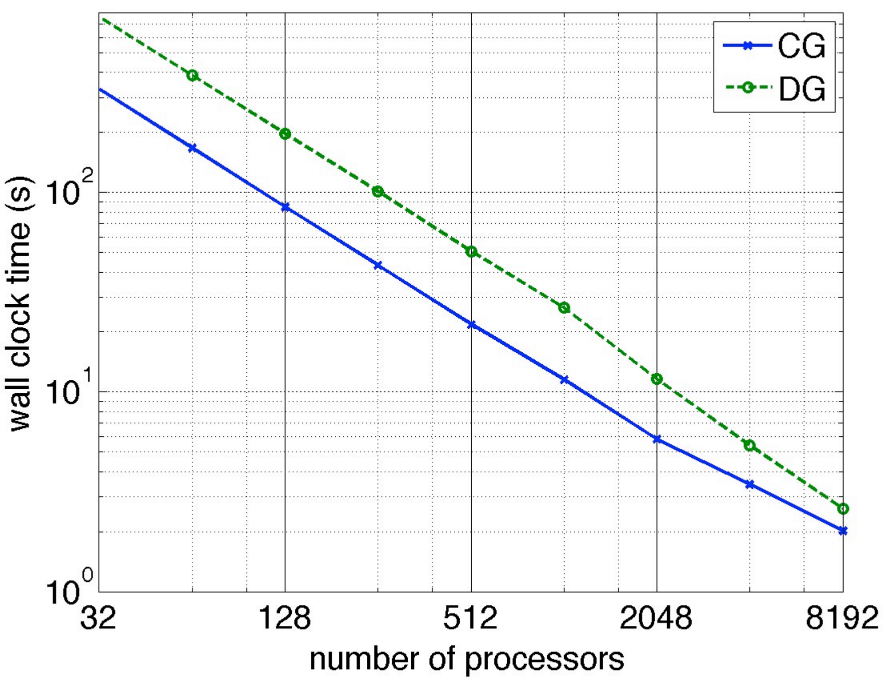
Talk Summary

1. New models need to exploit available computers
2. Numerical methods in new GFD models
3. Desired properties of our future GFD models
   - E.g., Conservation, Scalability, High-order Accuracy, Adaptivity
4. NUMA Model

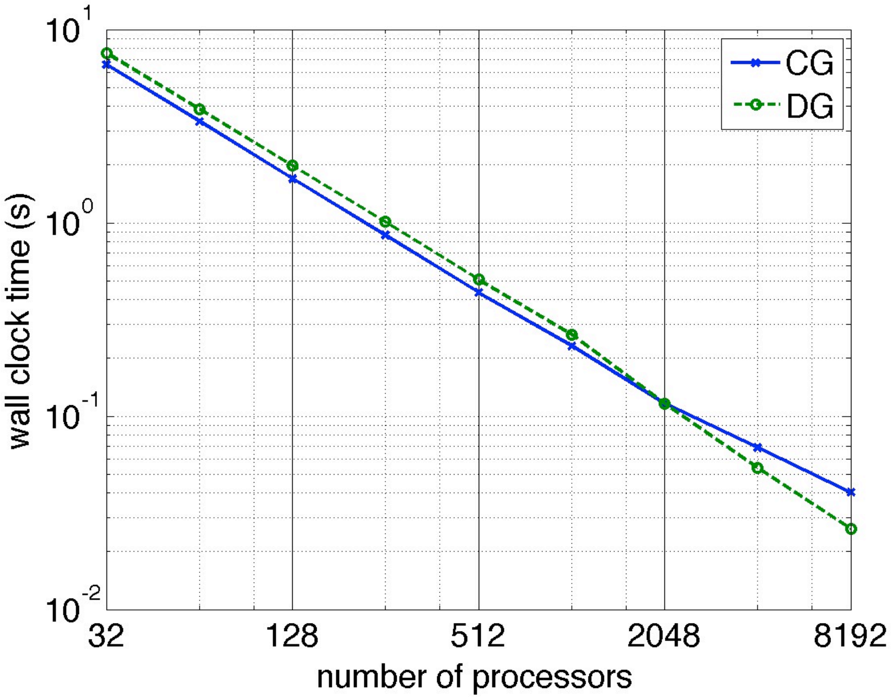
Desired Properties of Future GFD Models

1. Conservation – Conservation of Mass and Energy are absolute musts; what else should we conserve?
2. **Scalability** – New models must be highly scalable because we will continue to get more processors
3. High-Order Accuracy – Accuracy is important, of course, but how do we measure this and what order accuracy is sufficient? This question is coupled to the accuracy of the physics, data assimilation, etc. From the standpoint of scalability, high-order is good (hp methods = on-processor work is large but the communication footprint is small). This is also a good strategy for exploiting MPI/Open MP Hybrid and CPU/GPU paradigms.
4. **Adaptivity** – Adaptive methods have improved tremendously in the past decade and it may offer an opportunity to solve problems not feasible a decade ago but we need to identify these applications (e.g., hurricanes, storm-surge modeling, clouds?).

Scalability



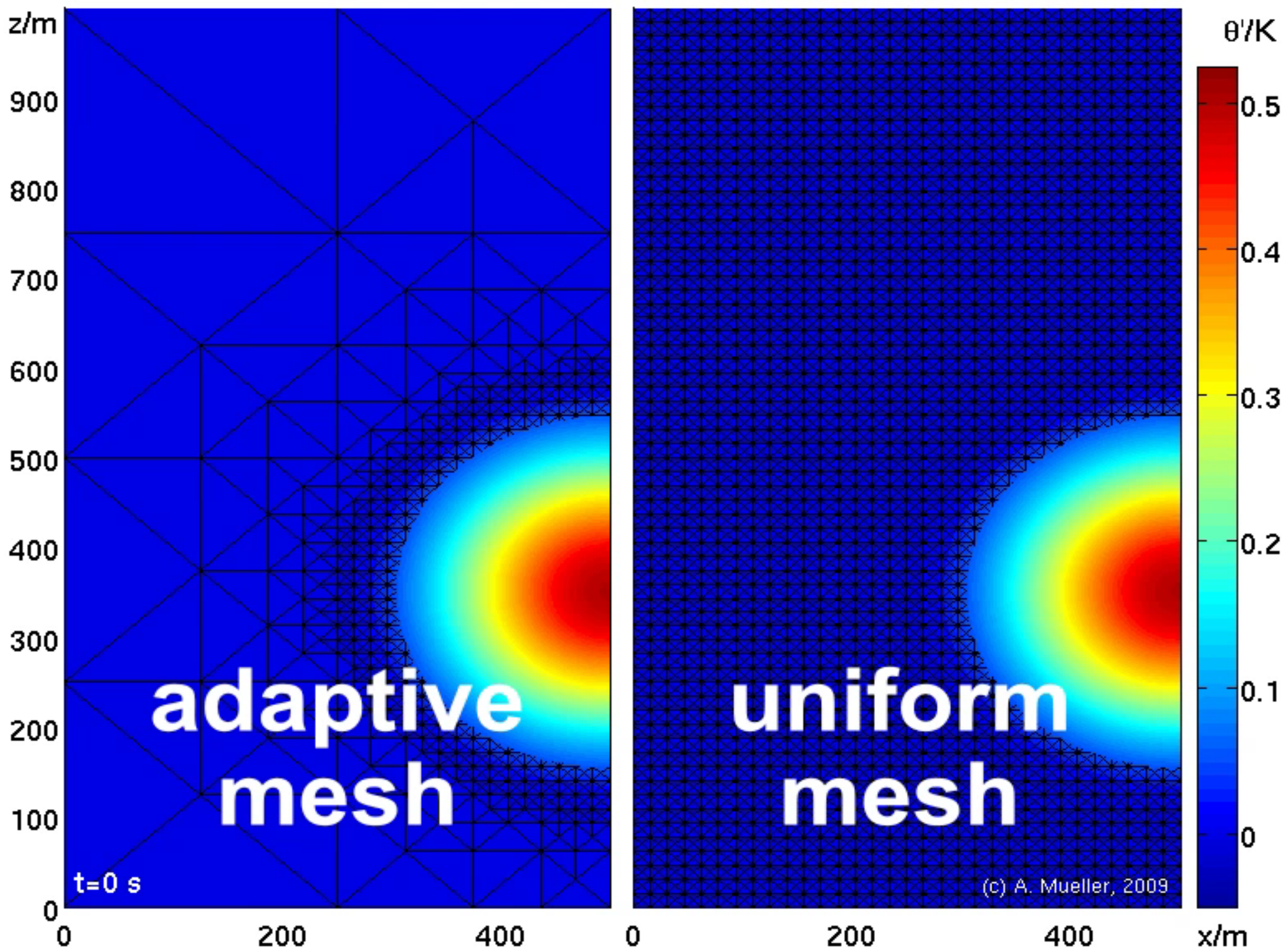
Total Cost



Cost Per Time-step

NUMA-CG and NUMA-DG with 16 Million Grid Points

Adaptivity
(Müller, Behrens, Giraldo, Wirth 2011)



Rising Thermal Bubble with Nonhydrostatic DG Model

Talk Summary

1. New models need to exploit available computers
2. Numerical methods in new GFD models
3. What should we aim for in our new models
4. NUMA Model
   - Design Philosophy
   - Governing Equations
   - Grids
   - Results

Design Philosophy

Unified Dynamics

- All limited-area models are nonhydrostatic. Resolutions of global models are approaching the nonhydrostatic limit (~10 km).
- Both limited-area and global models utilize the same equations.
- Engineer a common dynamical core (DyCore) for both models, then change grids and boundary conditions.

Unified Numerics

- CG is more efficient for smooth problems at low processor counts.
- DG is more accurate for problems with sharp gradients and more efficient at high processor counts.
- Both EBGs utilize a common mathematical arsenal.
- NUMA allows the user to choose either CG or DG for the problem at hand.

Unified Code

- Code is *modular*, with a common set of data structures.
- New time-integrators, grids, basis functions, physics, etc. may be swapped in and out with ease.
- Code is portable: Successfully installed on Apple, Sun, Cray, and IBM.

Governing Equations
(Unified Global/Mesoscale Equations)

Beginning with the Equations:

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \mathbf{u}) = 0$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \bullet \nabla \mathbf{u} + \frac{1}{\rho} \nabla P + g\hat{\mathbf{r}} + f(\hat{\mathbf{r}} \times \mathbf{u}) = 0$$

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \bullet \nabla \theta = 0$$

$$P = P_A \left(\frac{\rho R \theta}{P_A} \right)^{\gamma}$$

We introduce the General Splitting:

$$\rho(x,y,z,t) = \rho_0(x,y,z) + \rho'(x,y,z,t)$$

$$\theta(x,y,z,t) = \theta_0(x,y,z) + \theta'(x,y,z,t)$$

$$P(x,y,z,t) = P_0(x,y,z) + P'(x,y,z,t)$$

Governing Equations
(Unified Global/Mesoscale Equations)

The Reference Fields satisfy certain conditions, e.g.,:

$$\hat{\mathbf{r}} \cdot \nabla P_0 = -\rho_0 g$$

$$\frac{1}{\rho_0} \nabla P_0 + g\hat{\mathbf{r}} + f\left(\hat{\mathbf{r}} \times \mathbf{u}\right) = 0$$

The following General Equations satisfy such conditions:

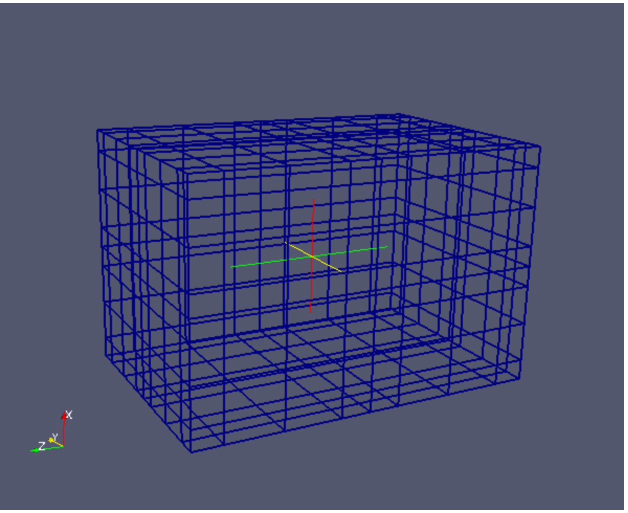
$$\frac{\partial \rho'}{\partial t} + \nabla \bullet \left(\rho \mathbf{u}\right) = 0$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \bullet \nabla \mathbf{u} + \frac{1}{\rho}\left(\mathbf{H}\nabla P_0 + \nabla P' + \rho' g\hat{\mathbf{r}}\right) = -f\left(\hat{\mathbf{r}} \times \mathbf{u}\right)$$

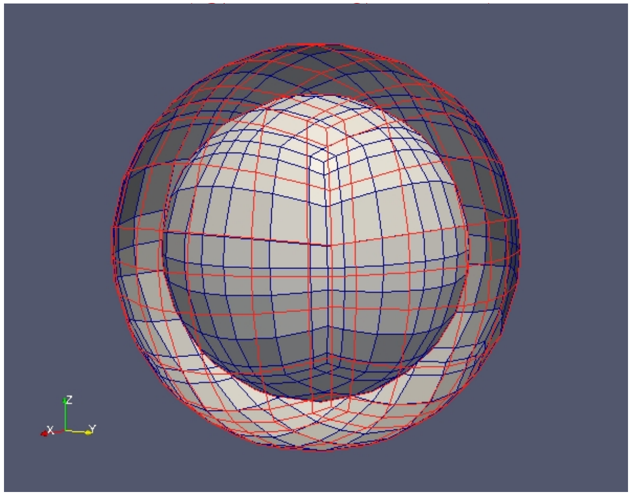
$$\frac{\partial \theta'}{\partial t} + \mathbf{u} \bullet \nabla \theta = 0$$

Grids

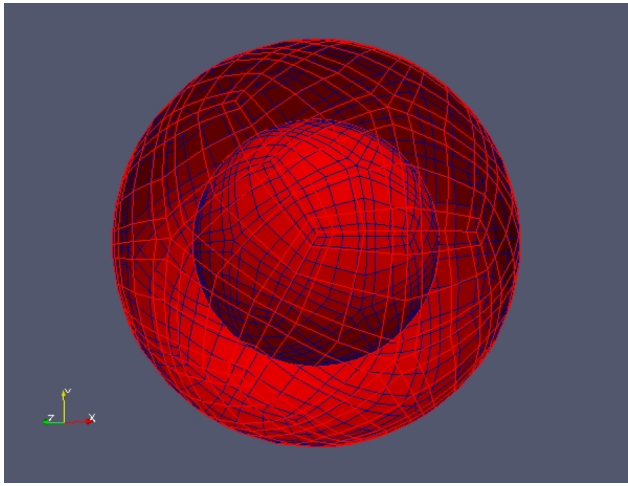
Mesoscale Modeling Mode

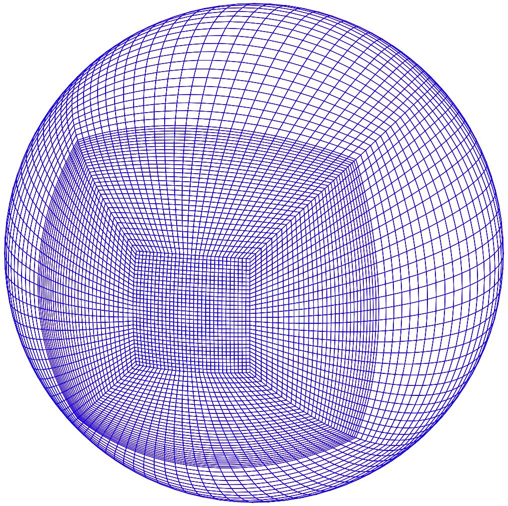


Global Modeling Mode

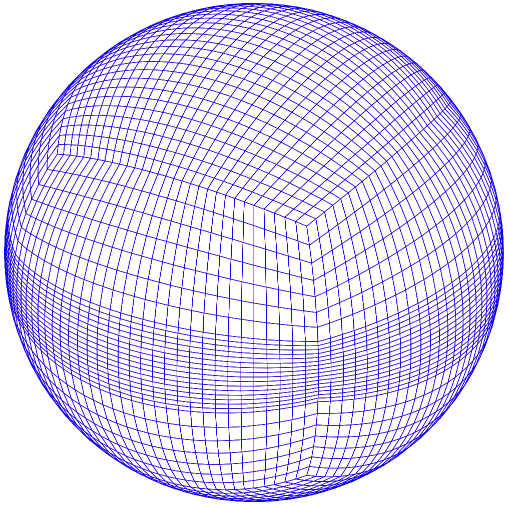


Global Modeling Mode (Icosahedral)





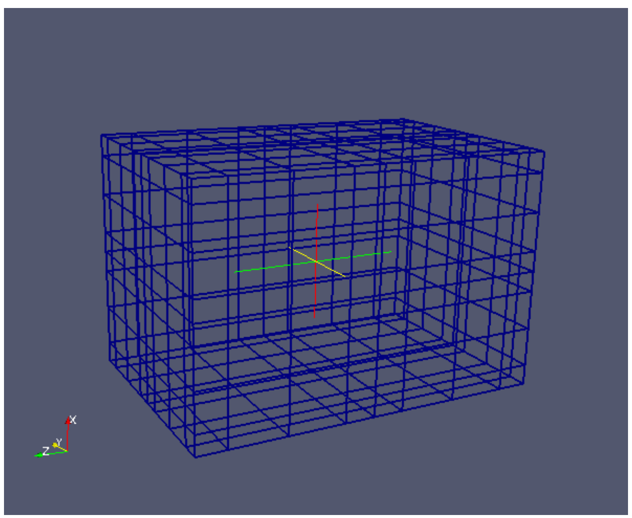
Telescoping Grid



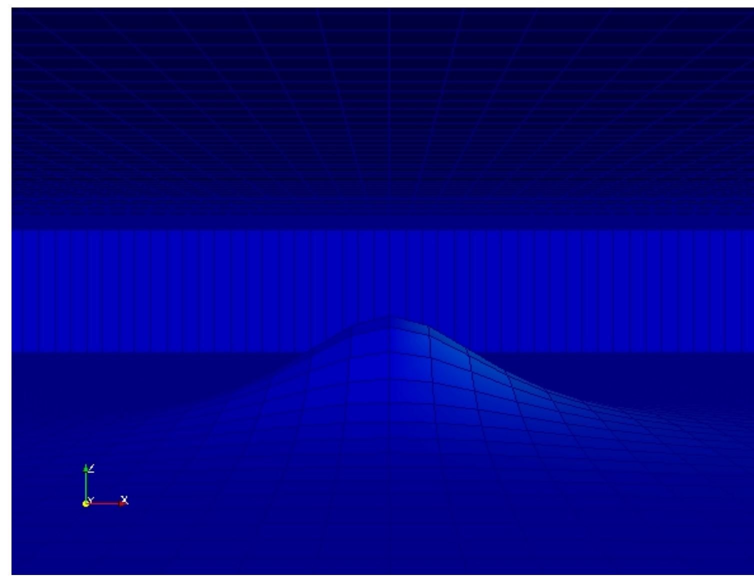
ITCZ Grid

Results: Mesoscale Mode
(3D Linear Hydrostatic Isolated Mountain)

- Flow of U=20 m/s in an isothermal atmosphere.
- LH Mountain: Solid of revolution of Witch of Agnesi: Mountain height = 1 m with radius 10 km.
- Absorbing (sponge) boundary condition implemented on lateral and top boundaries.

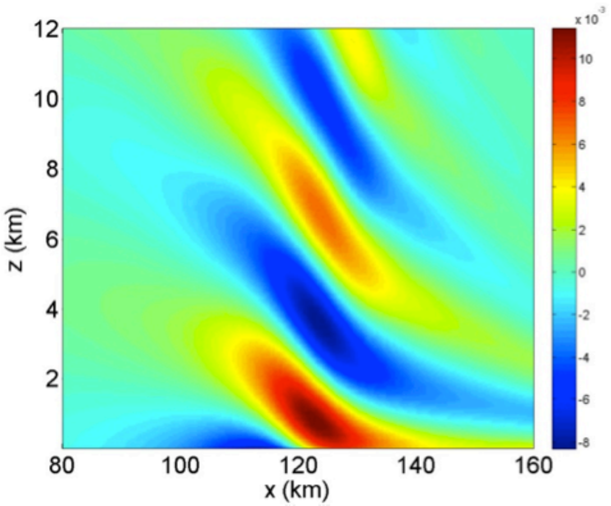


Grid

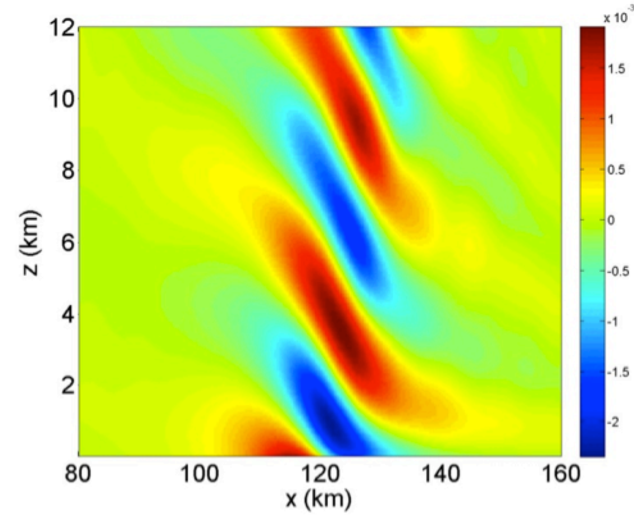


Geometry

3D Linear Hydrostatic Isolated Mountain
(T=1 hour)

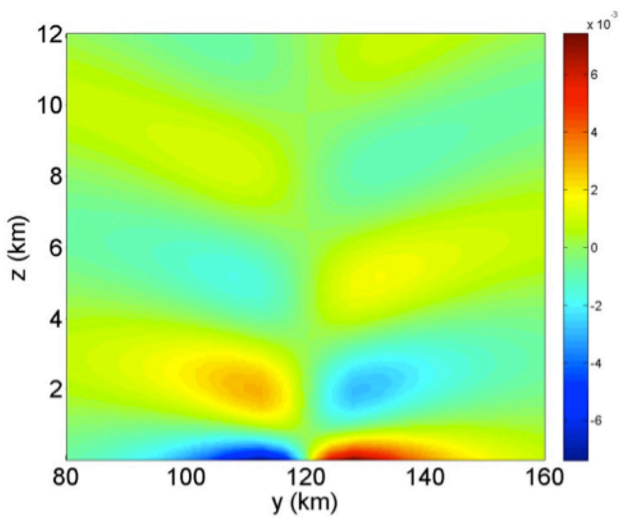


u

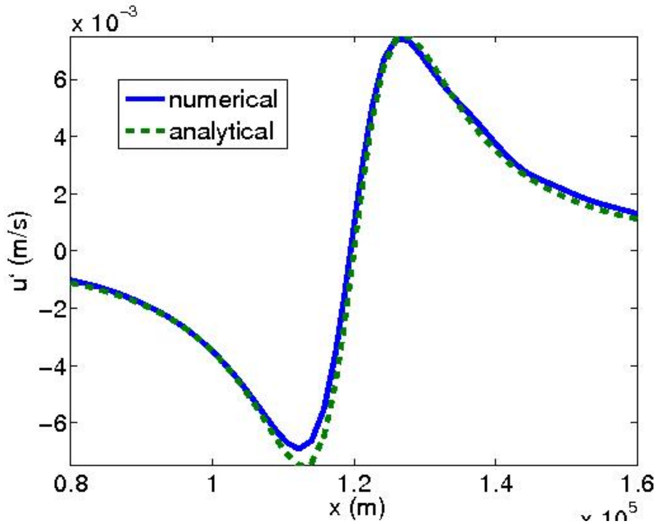


w

v

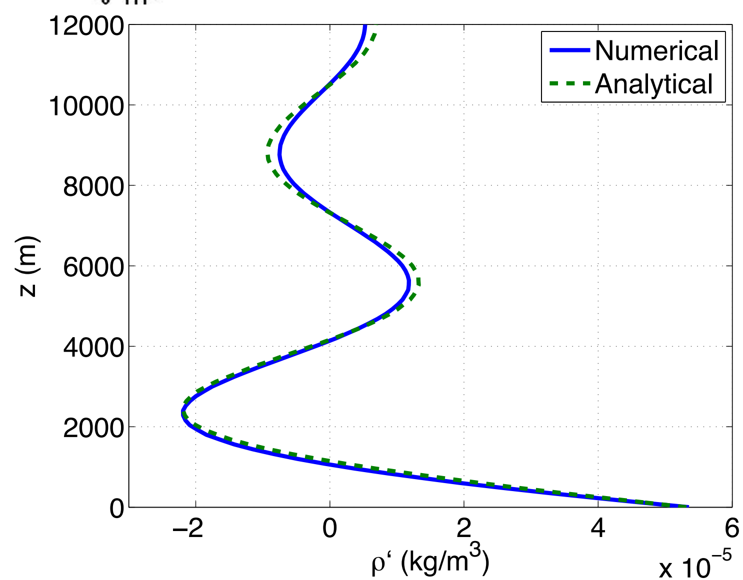


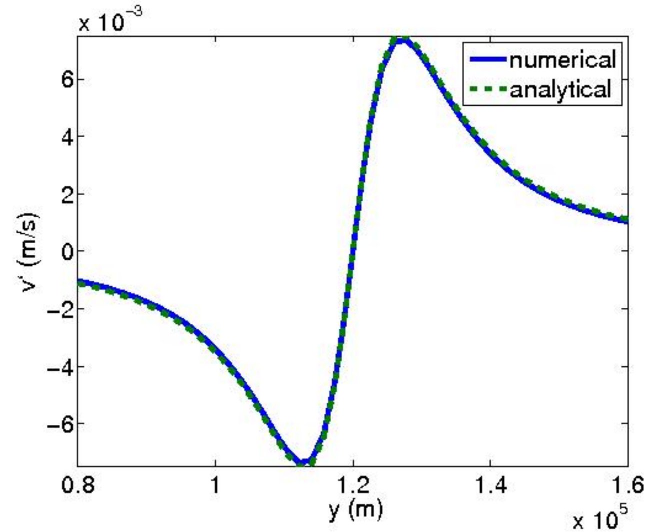
3D Linear Hydrostatic Isolated Mountain (T=1 hour)



u

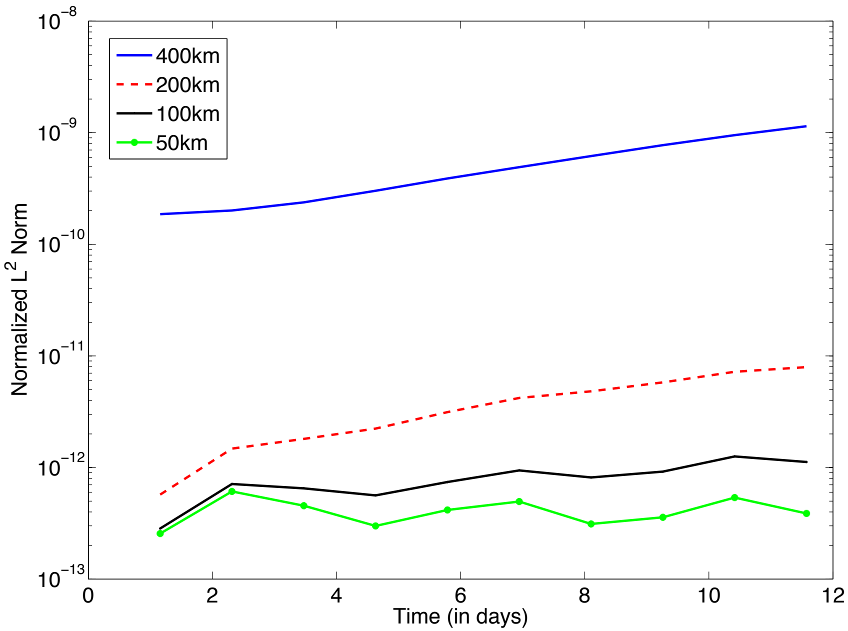
rho

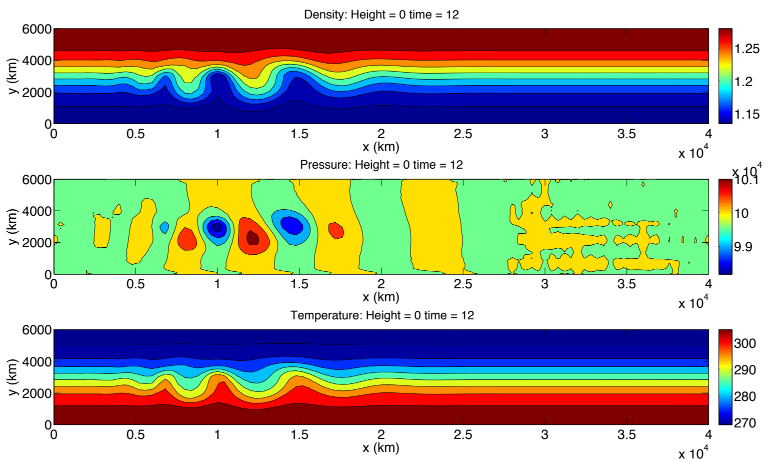




v

Results: Mesoscale Mode
(Balance Initial State and Baroclinic Instability)

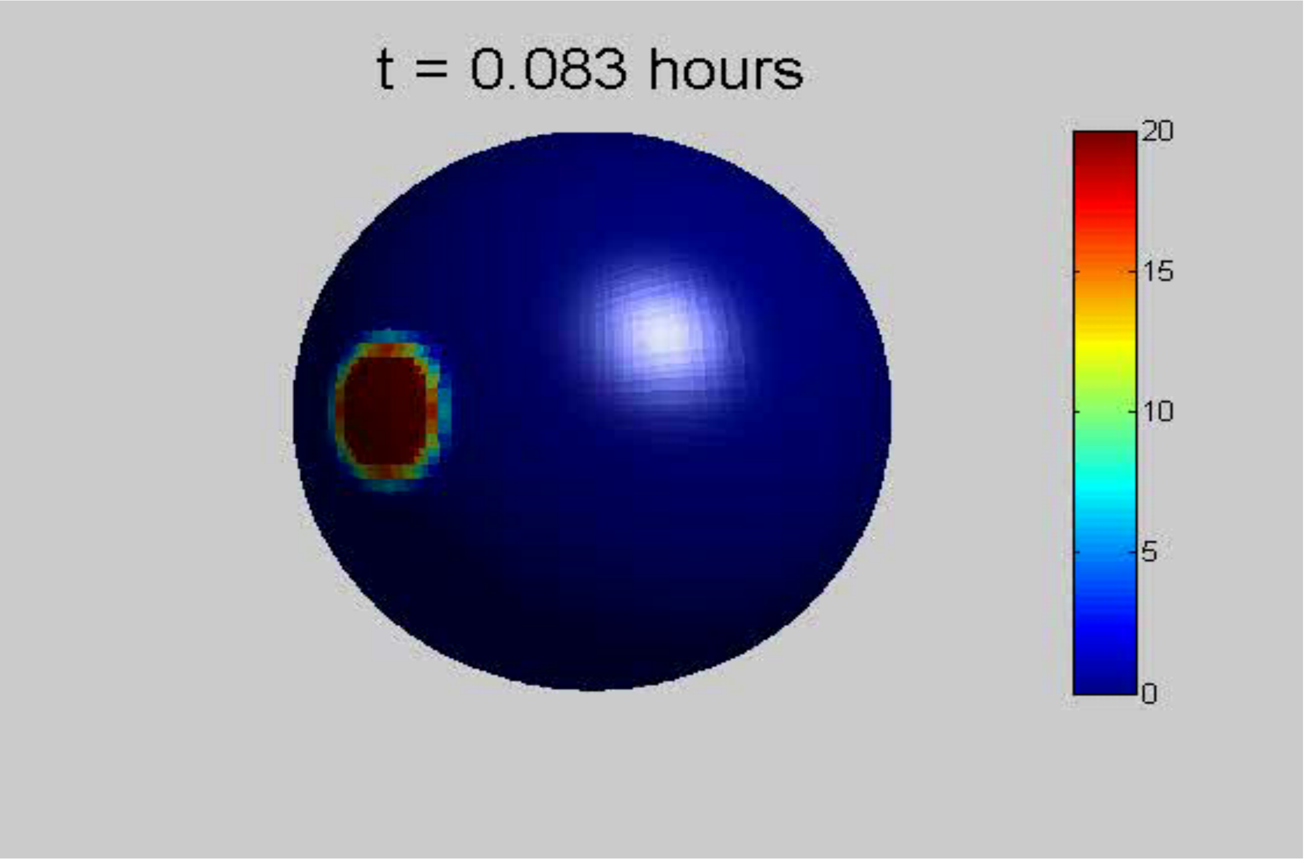




Balanced Initial State (Hydrostatically and Geostrophically balanced)

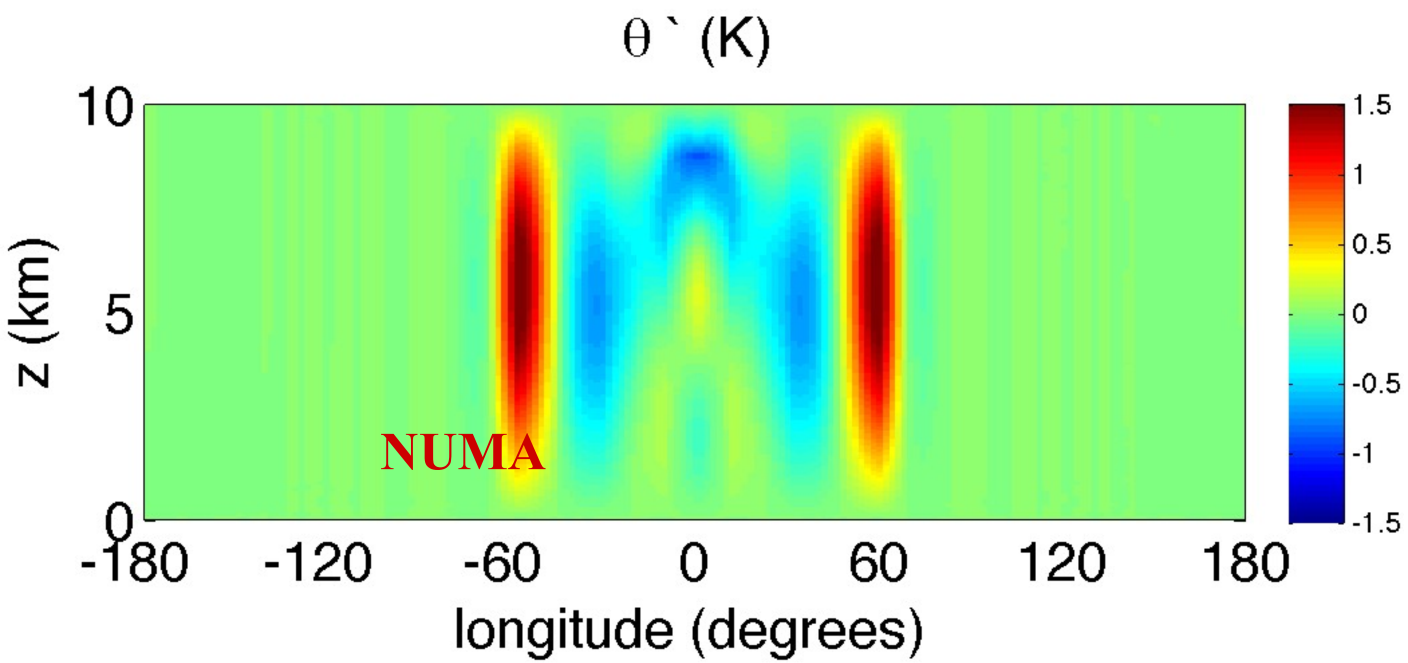
Baroclinic Instability

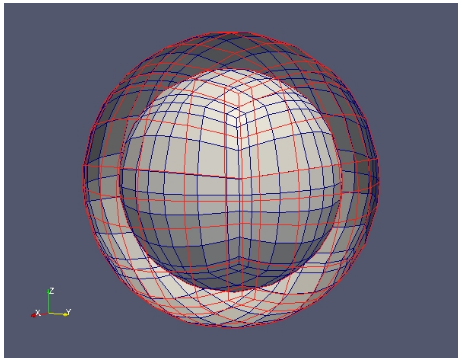
Results: Global Mode
(Planetary Acoustic Wave Propagation)



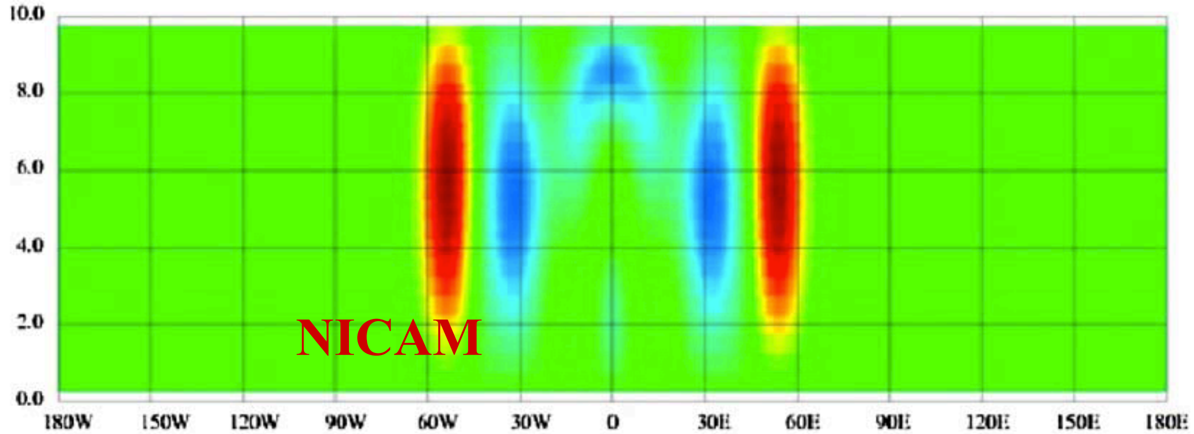
Theory=347 m/s,
NUMA model=347 m/s,
NICAM model = 338 m/s

Results: Global Mode
(Inertia-Gravity Wave Propagation N=0.01, T=48 hours)



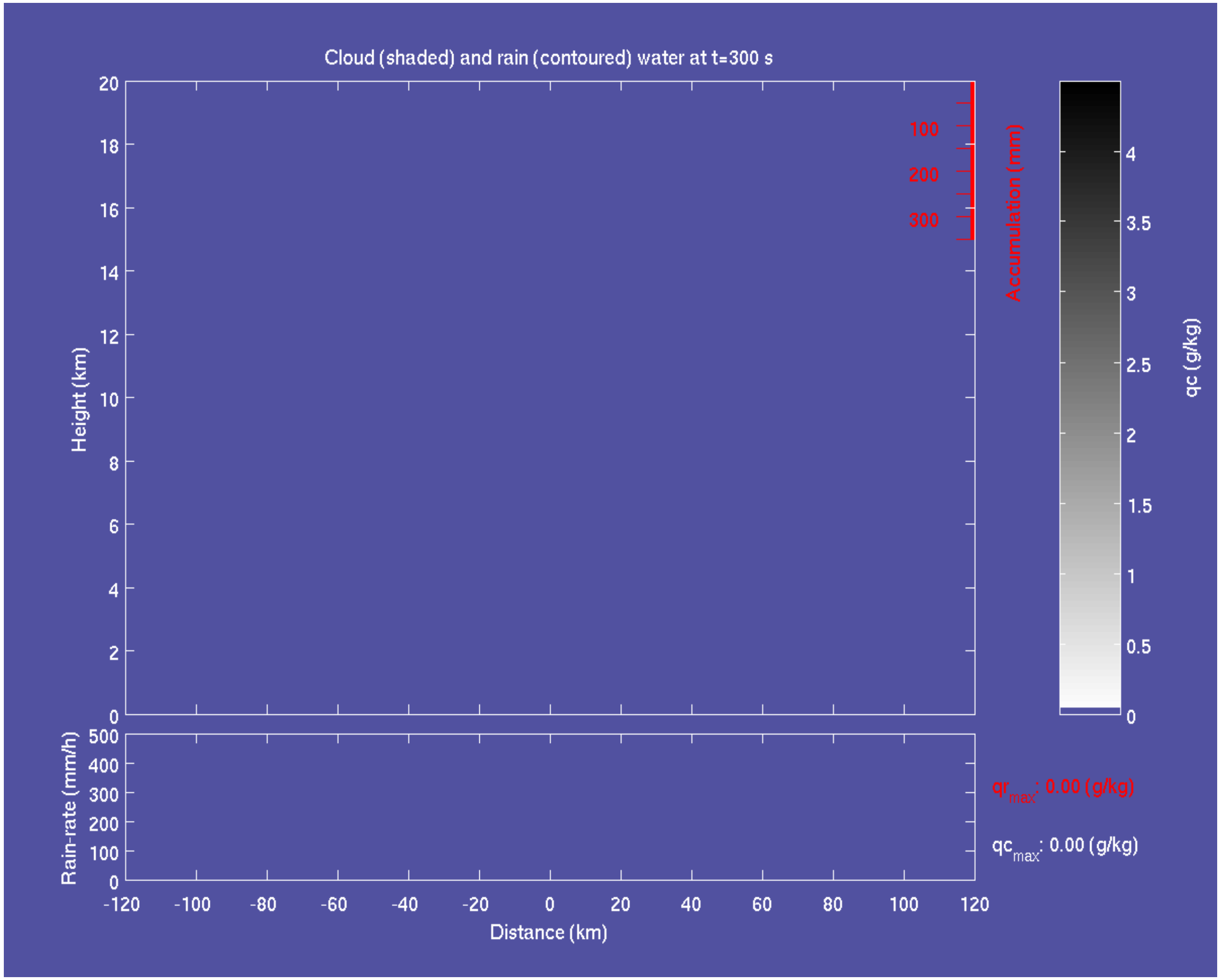


Grid



Theory=32 m/s,
NUMA model=33 m/s,
NICAM model = 33 m/s

NUMA2D Simple Moist Physics (Mesoscale)



A Multitude of Challenges Remain

- Continuous and Discontinuous Galerkin methods are good choices for hydrostatic and non-hydrostatic atmospheric models.
- The NUMA dynamical core is quite mature:
  - 3D and MPI (Kelly and Giraldo JCP 2011) .
  - Can use either CG or DG methods.
  - Contains a suite of IMEX time-integrators (Giraldo et al. SISC 2011).
  - Has been verified on a variety of limited-area and global tests.
- The NUMA physics is under development:
  - Simple sub-grid scale parameterization has been added to NUMA2D (Gabersek et al. MWR 2011).
  - Variational Multi-scale (VMS) method is being added to NUMA2D with physics for positivity of tracers (Marras et al. JCP 2011).
  - Simple physics being added to NUMA3D along with VMS algorithm.

A Multitude of Challenges Remain

- Future Projects:
  - Conduct a variety of verification and validation simulations.
  - Add IMEX methods to NUMA-DG (currently only in NUMA-CG part).
  - Study and Implement Multi-Rate (Patrick Mugg Thesis).
  - Explore new Riemann solvers for NUMA-DG (Maria Lukacova)
  - Develop adaptive methods for unified limited-area/global modeling simulations (work in progress by Kopera and Gopalakrishnan, NPS)
  - NUMA is being coupled with PETSc – ANL (DoE ASCR program) has chosen NUMA as its flagship application.