2012 American Geophysical Union Fall Meeting:

High resolution three-dimensional modeling with an adaptive grid regional-scale air quality model

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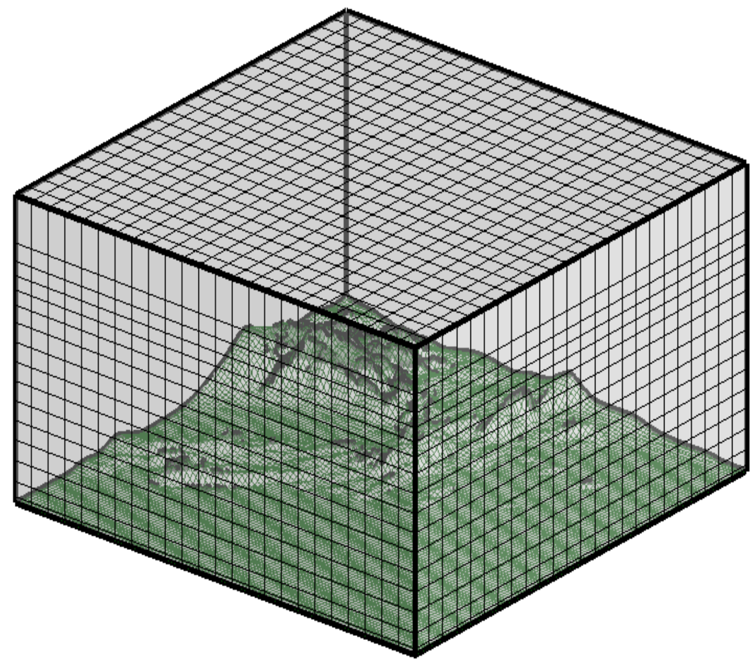
Modeling Pollution Plumes with Eulerian Air Quality Models

Advantages:

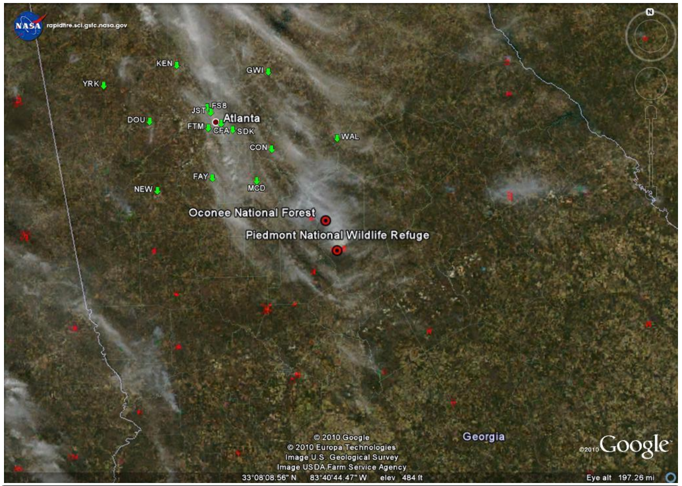
- State-of-the-science representations of complex physical and chemical processes
- Comprehensive emissions inventories
- Detailed 3-dimensonal meteorological fields

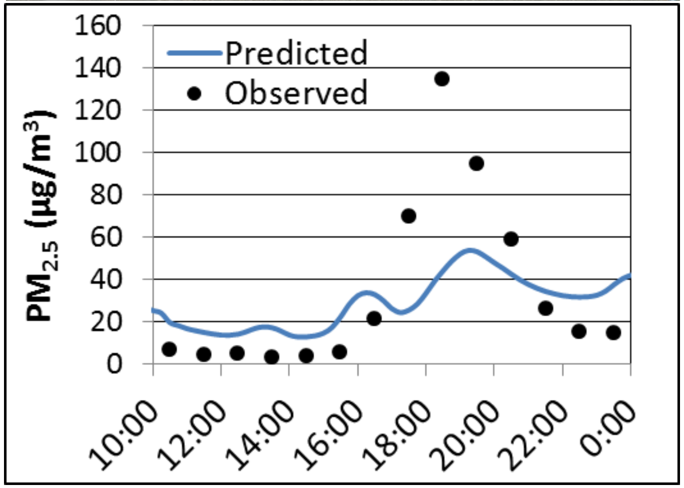


Multiscale capabilities :

- Initial transformations and dispersion
  → local scales
- Long-range transport and air quality impact
  → regional and global scales

Modeling Pollution Plumes with Eulerian Air Quality Models





Limitations:

- Immediate dilution of emissions
- Numerical diffusion
- Errors in non-linear transformations
- Parameterization or omission of subgrid scale processes

Observations from Plume Simulations:

- Regional-scale models can be ineffective as a prediction tool for pollutant plumes
- Severely underpredicted AQ impacts
- Significant sensitivity of modeled concentrations to grid resolution

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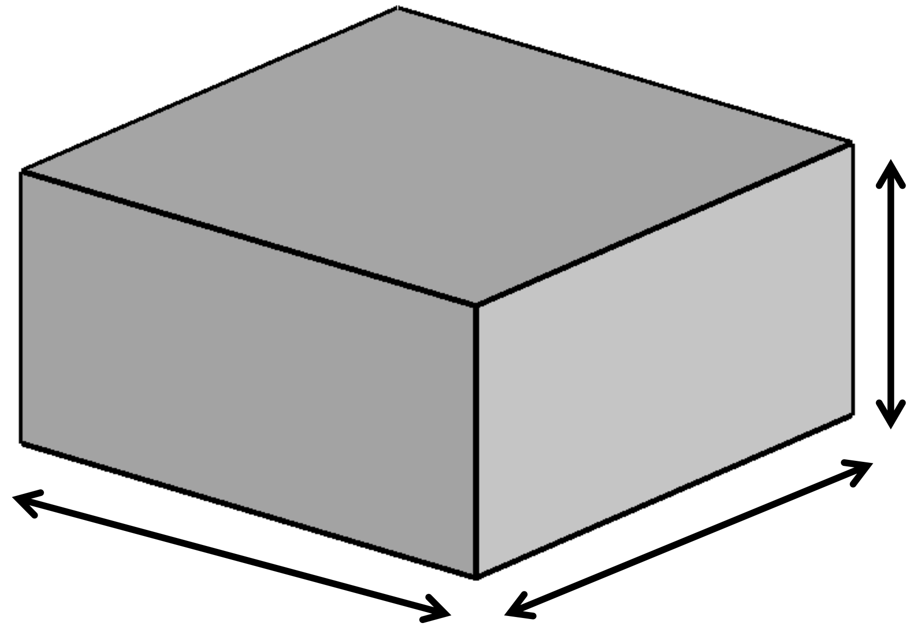
OBJECTIVE: *Develop a three-dimensional modeling technique that will allow simulations of atmospheric plumes with unprecedented resolution using gridded air quality models*



OBJECTIVE: *Develop a three-dimensional modeling technique that will allow simulations of atmospheric plumes with unprecedented resolution using gridded air quality models*

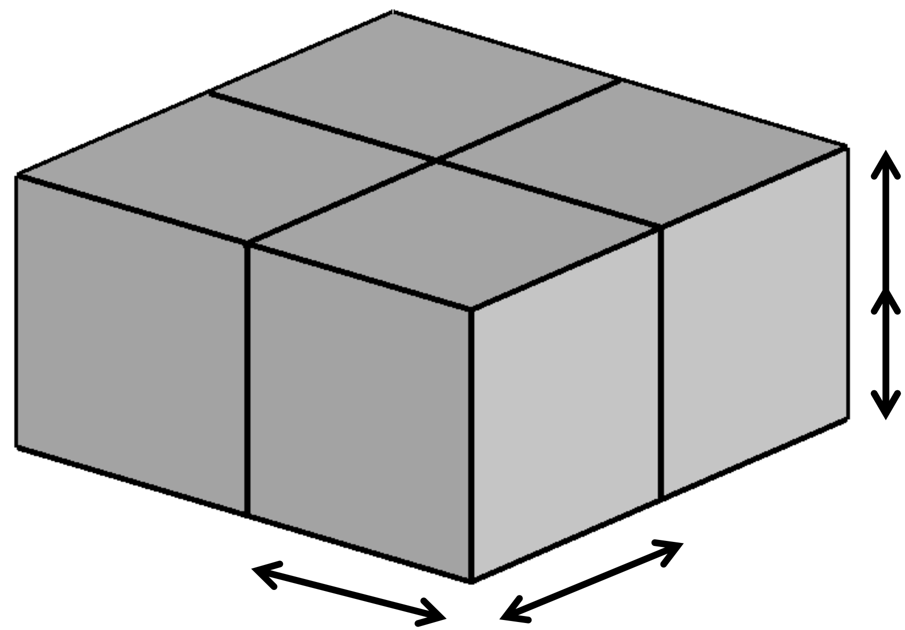
Computational Demand:

2x horizontal resolution:

4x N → 4-16x operations

2x horizontal & vertical resolutions:

8x N → 8-64x operations



Stability considerations:

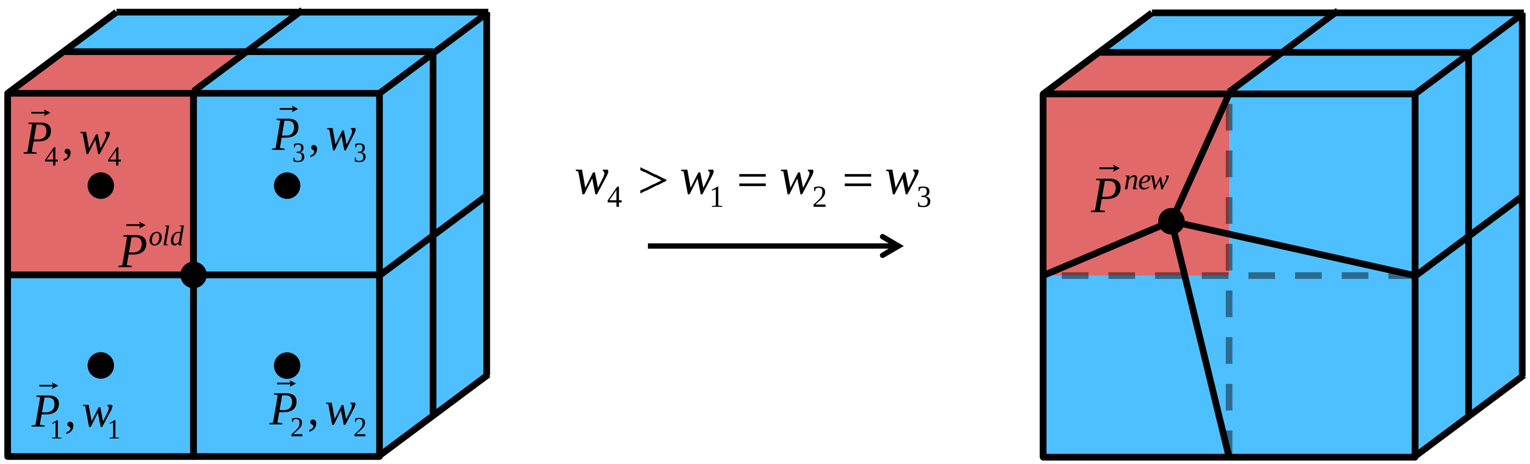
$\Delta t = \Delta x / u$ $\Delta x \downarrow \rightarrow \Delta t \downarrow$

2x resolution → 2x operations

Adaptive Grid Algorithm

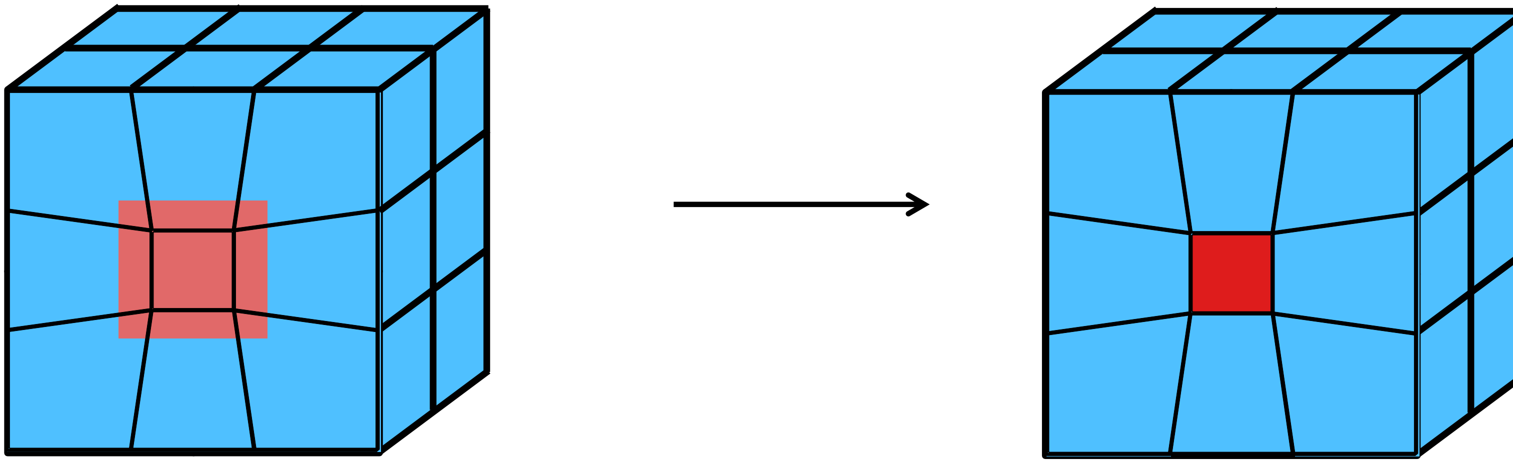
1. Assign a weight to each cell: $$w = \sum_n \alpha_n \nabla^2 c_n$$

2. Use cell weights to estimate new node positions: $$\vec{P}_i^{new} = \sum_{k=1}^{8} w_k \vec{P}_k \Big/ \sum_{k=1}^{8} w_k$$



Adaptive Grid Algorithm

3. Redistribute concentration fields:

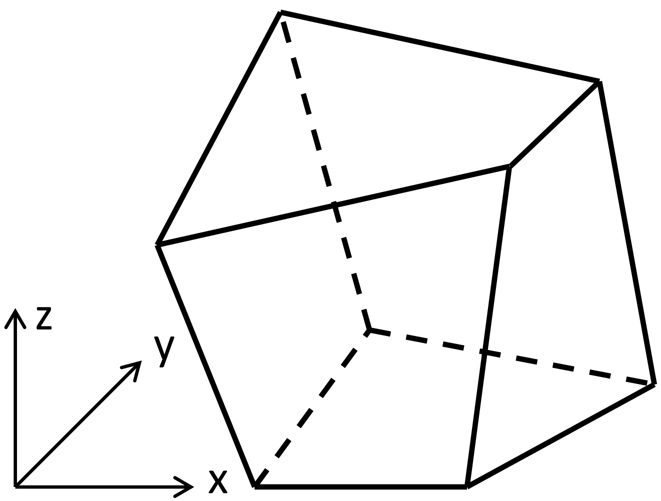


4. Check convergence criteria:

   → node movement < 5% internodal distance

Coordinate Transformation

Physical Domain



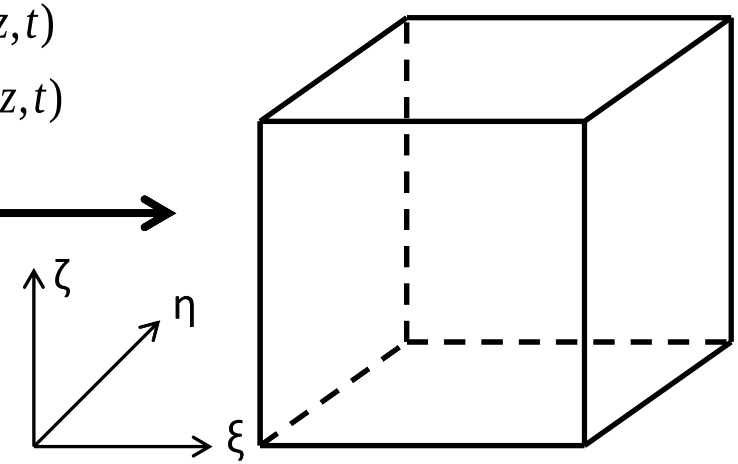
$$\xi = \xi(x, y, z, t)$$

$$\eta = \eta(x, y, z, t)$$

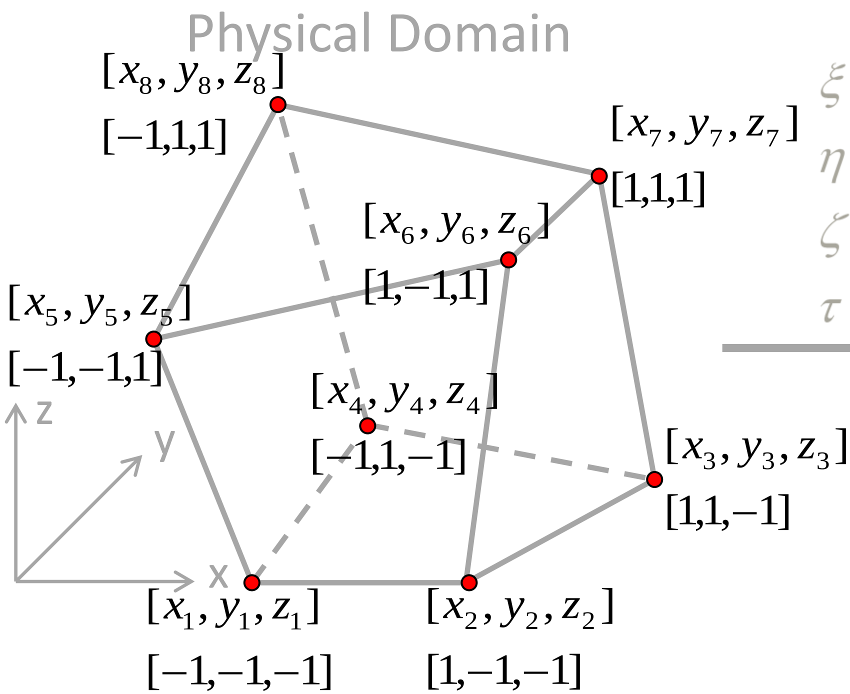
$$\zeta = \zeta(x, y, z, t)$$

$$\tau = t$$

Computational Domain



Coordinate Transformation



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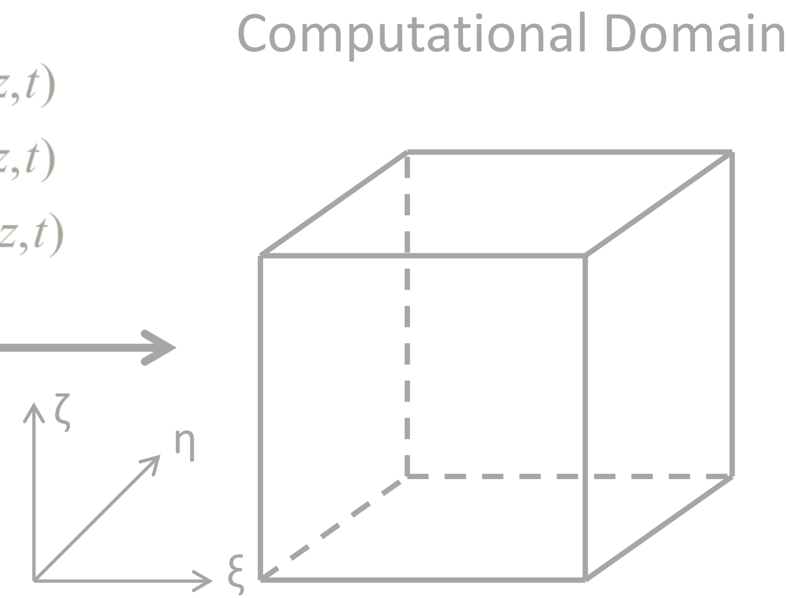
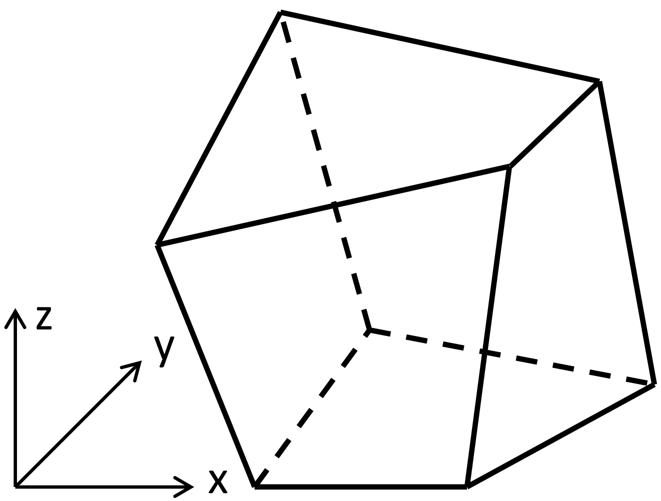


$$(x, y, z) \leftrightarrow (\xi, \eta, \zeta)$$

Coordinate Transformation

Physical Domain

Computational Domain



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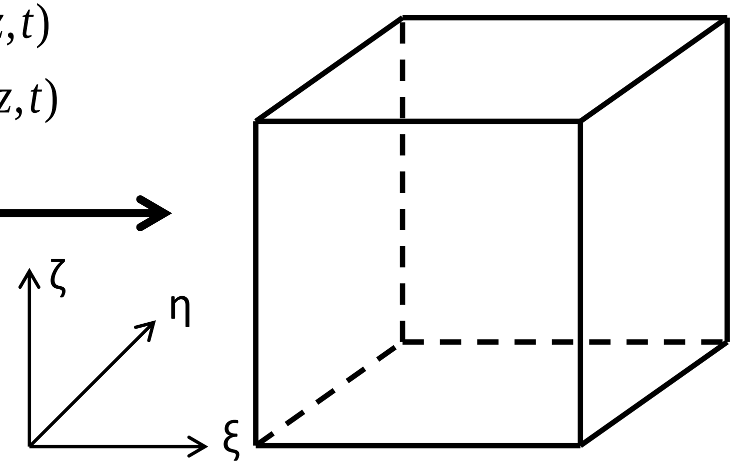
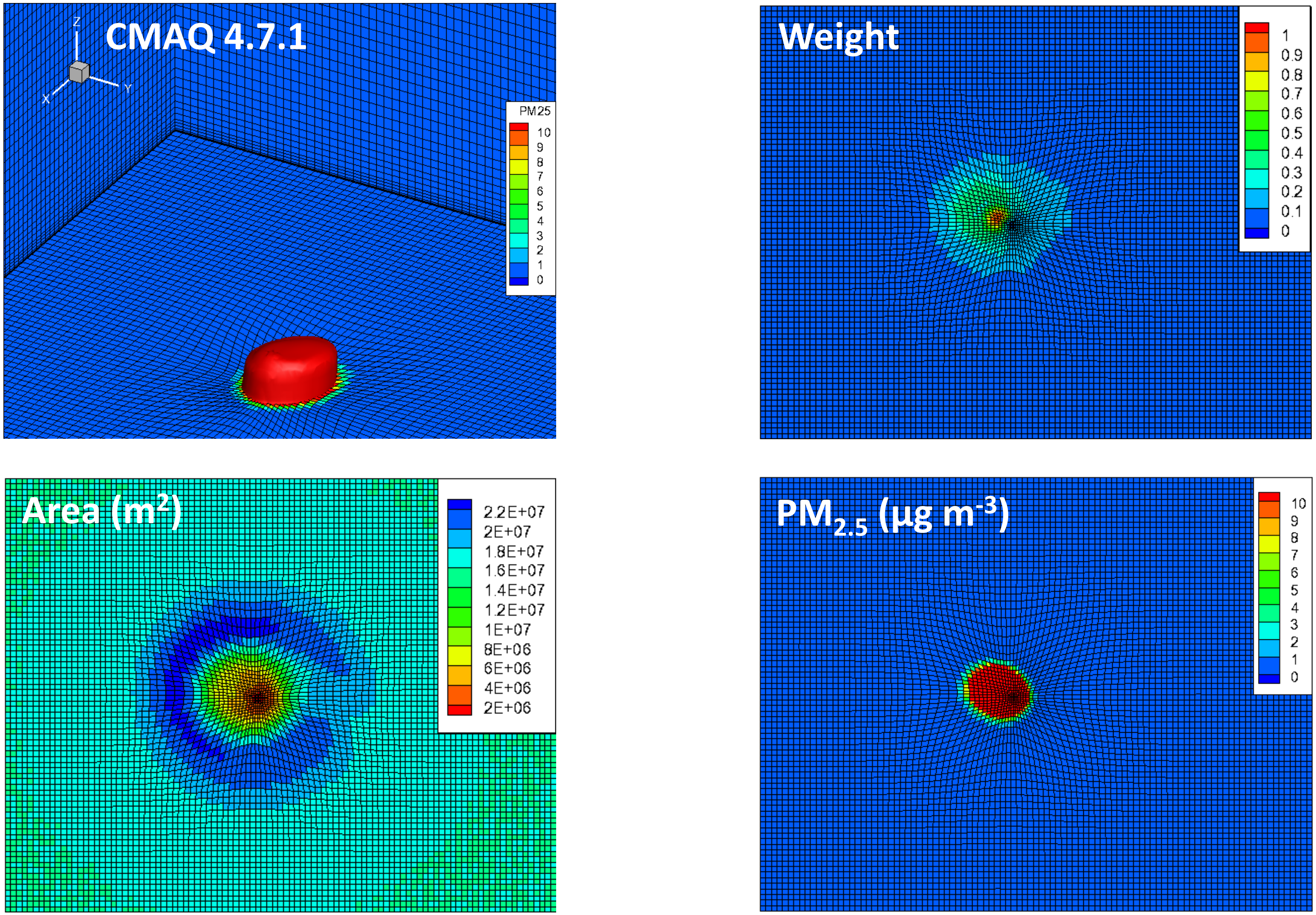


$$\frac{\partial C}{\partial t}+\frac{\partial (uC)}{\partial x}+\frac{\partial (vC)}{\partial y}+\frac{\partial (wC)}{\partial z} +\frac{\partial}{\partial x}\left(K^{xx}\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(K^{yy}\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(K^{zz}\frac{\partial C}{\partial z}\right)=R+S$$

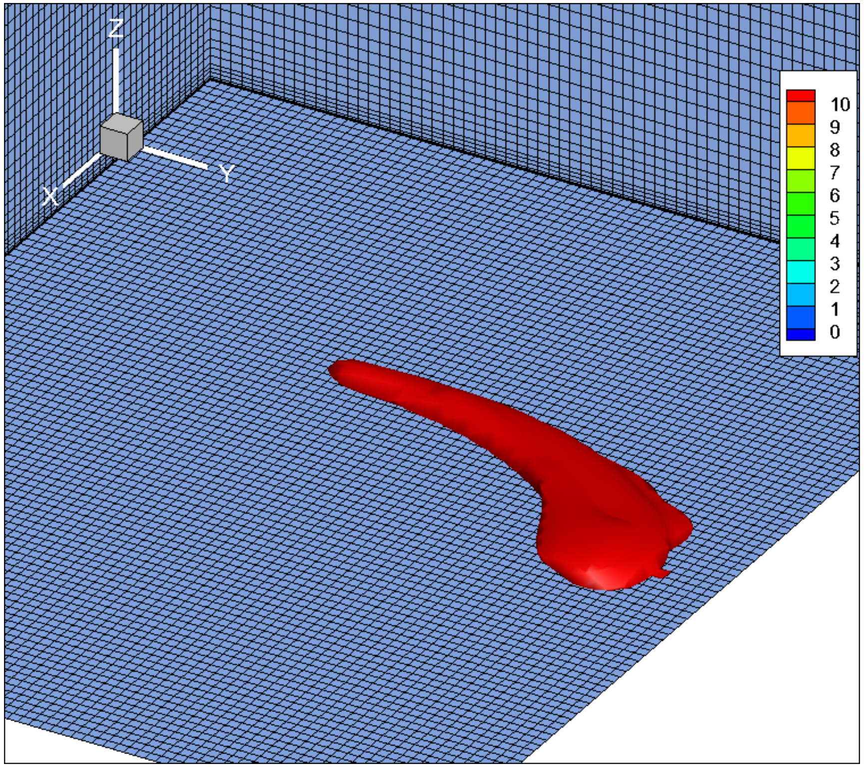
$$\frac{\partial (J^{-1}C)}{\partial \tau}+\frac{\partial (J^{-1}C)}{\partial \xi}\frac{\partial \xi}{\partial t}+\frac{\partial (J^{-1}C)}{\partial \eta}\frac{\partial \eta}{\partial t}+\frac{\partial (J^{-1}C)}{\partial \zeta}\frac{\partial \zeta}{\partial t}+\frac{\partial (J^{-1}v^{\xi}C)}{\partial \xi}+\frac{\partial (J^{-1}v^{\eta}C)}{\partial \eta}+\frac{\partial (J^{-1}v^{\zeta}C)}{\partial \zeta} +\frac{\partial}{\partial \xi}\left(J^{-1}K^{\xi\xi}\frac{\partial C}{\partial \xi}\right)+\frac{\partial}{\partial \eta}\left(J^{-1}K^{\eta\eta}\frac{\partial C}{\partial \eta}\right)+\frac{\partial}{\partial \zeta}\left(J^{-1}K^{\zeta\zeta}\frac{\partial C}{\partial \zeta}\right)=J^{-1}R+J^{-1}S$$

2-D Implementation in CMAQ

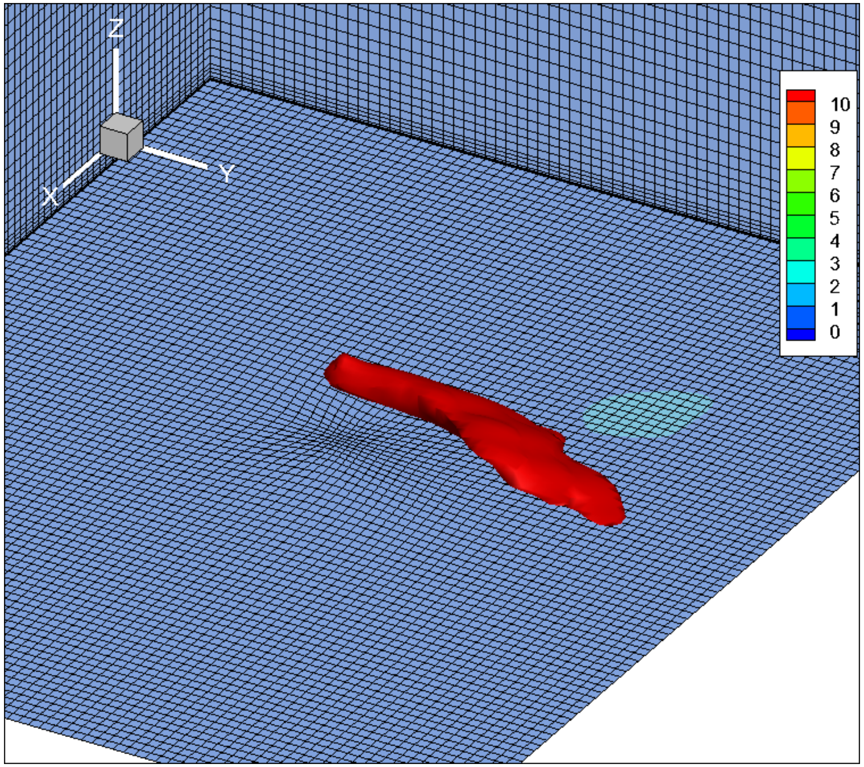


Adaptive Grid Tests in CMAQ

Fixed Grid



Adaptive Grid



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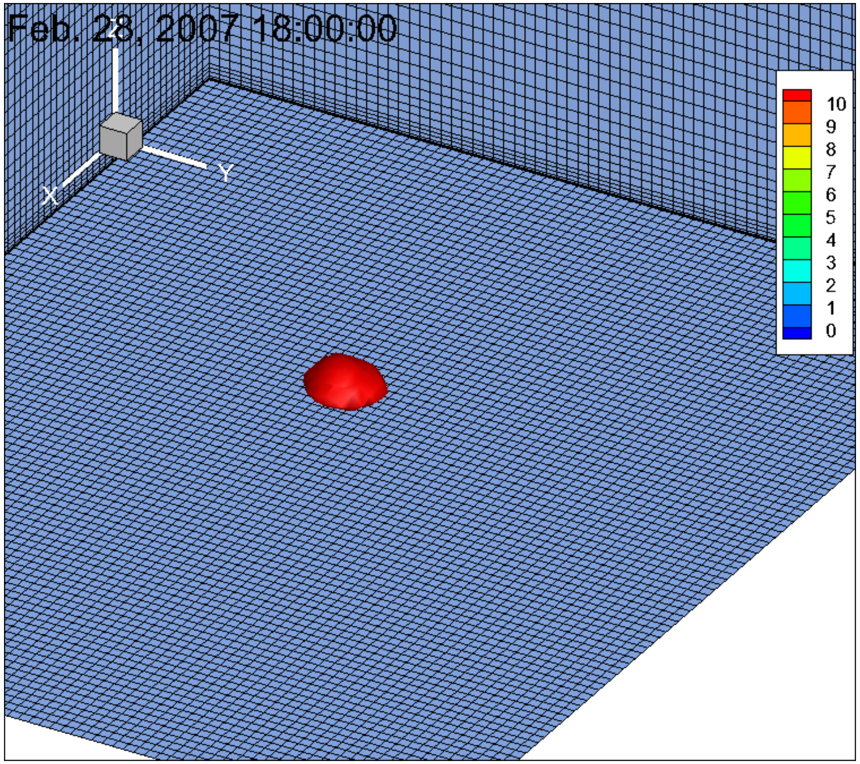
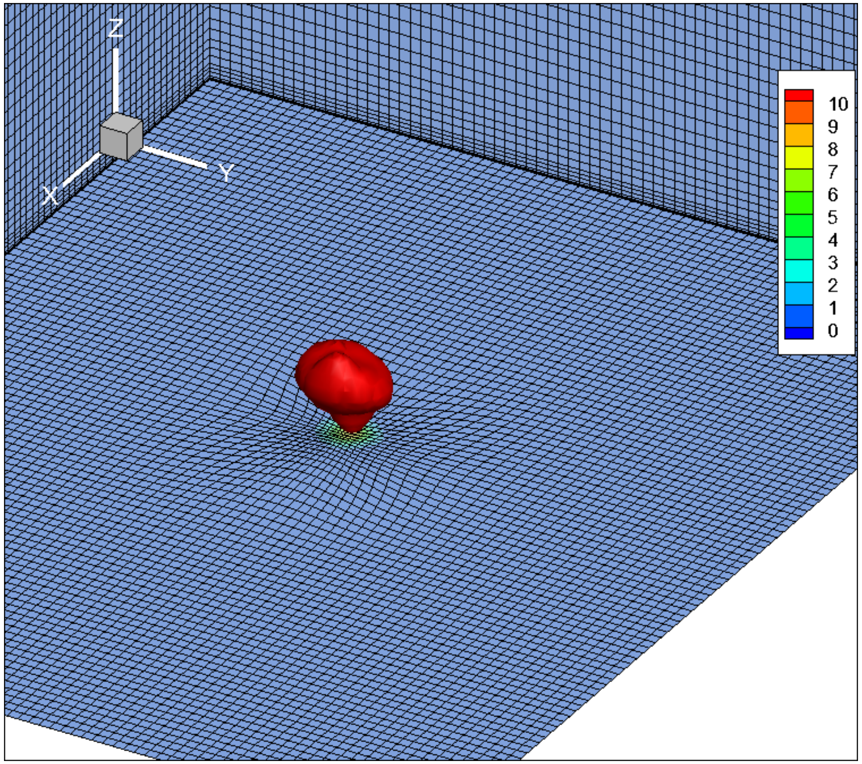
Adaptive Grid Tests in CMAQ

Fixed Grid



Adaptive Grid



Adaptive Grid Tests in CMAQ

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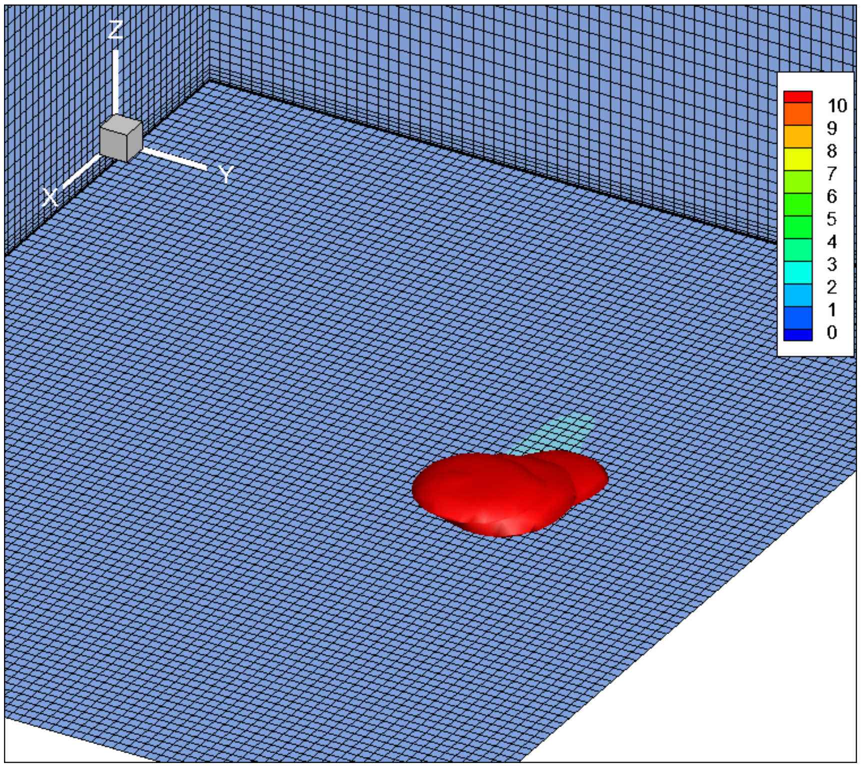
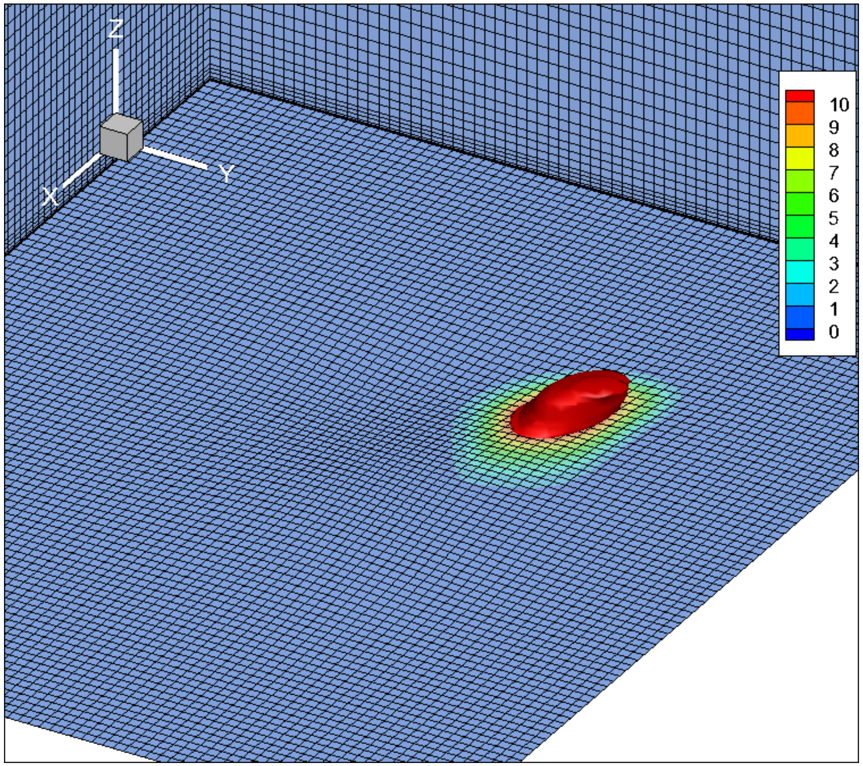
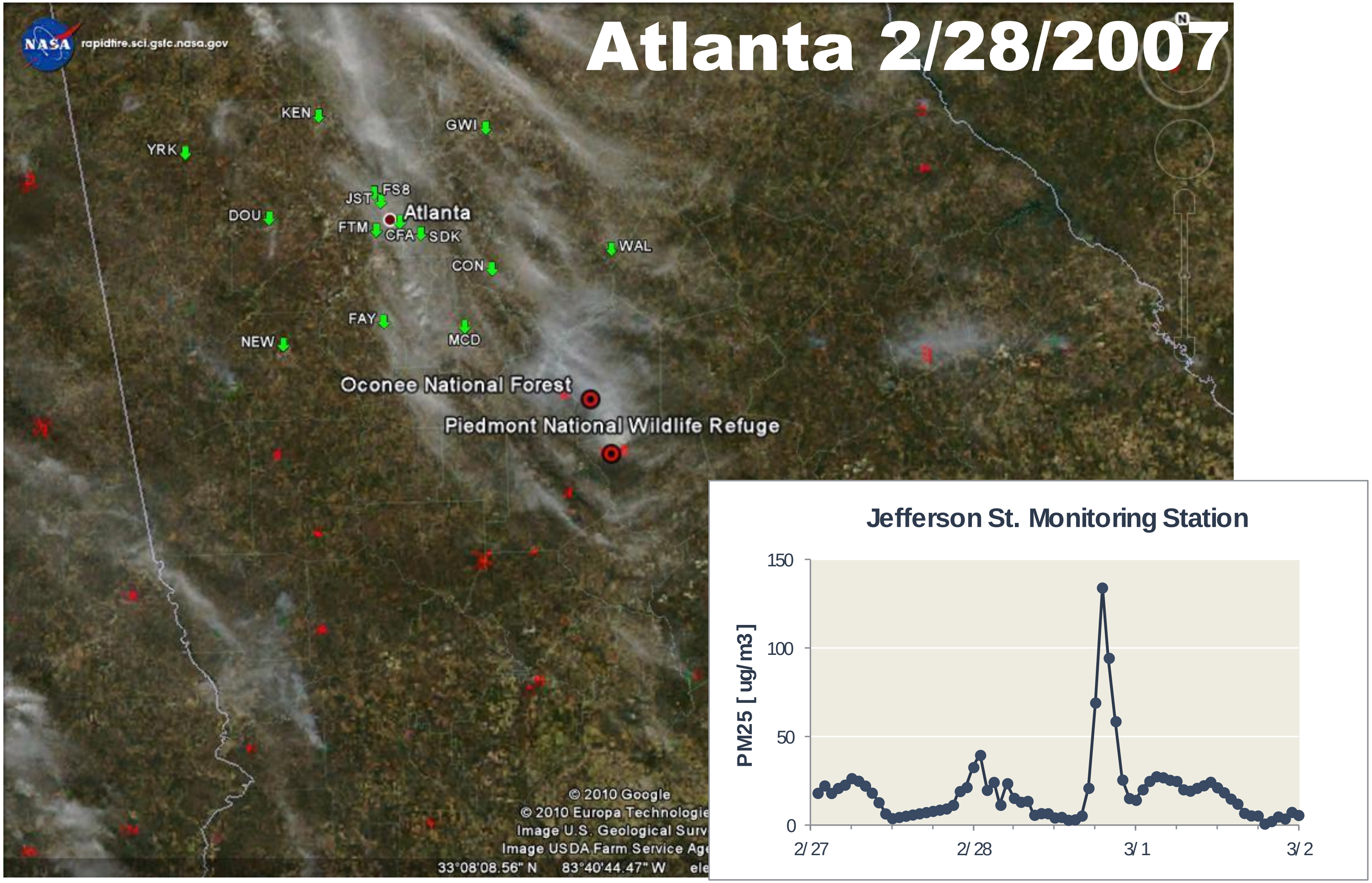


Adaptive Grid



Adaptive Grid Evaluation in CMAQ



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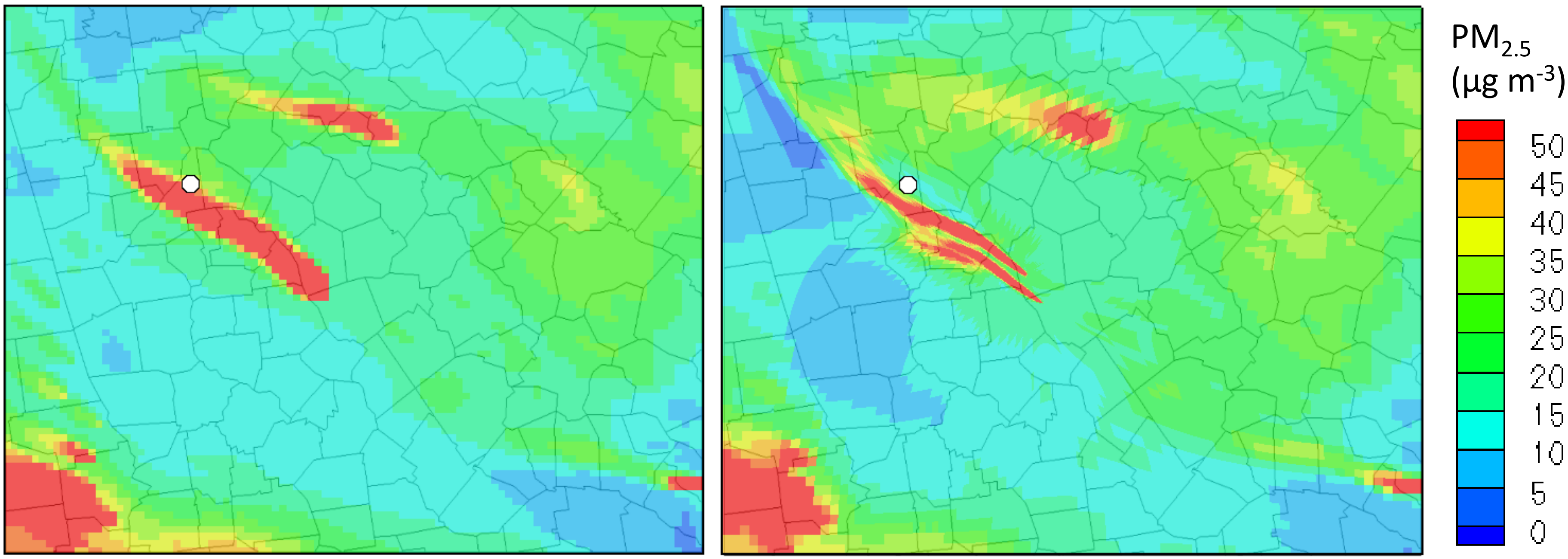
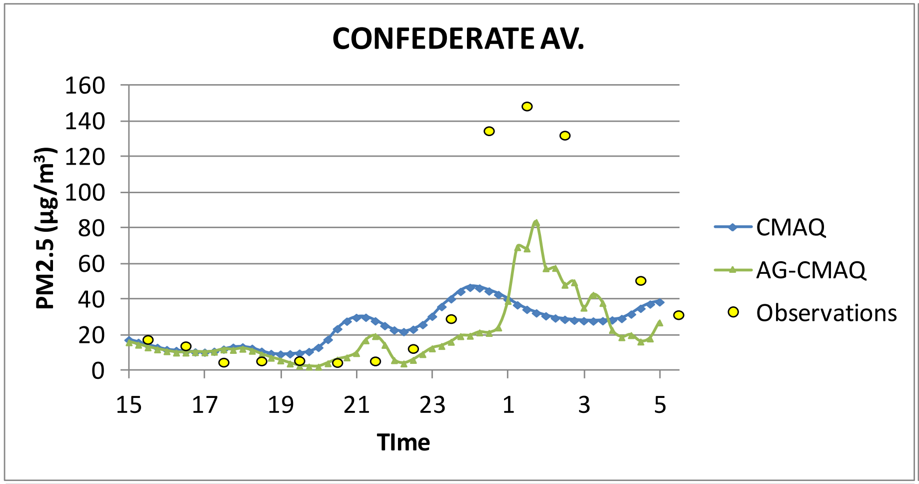
Adaptive Grid Evaluation in CMAQ

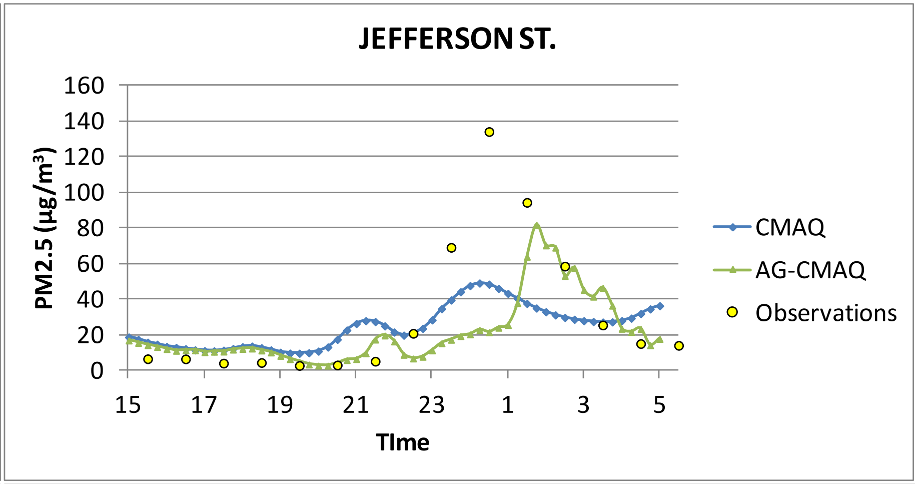
Fixed Grid (4km) | Adaptive Grid

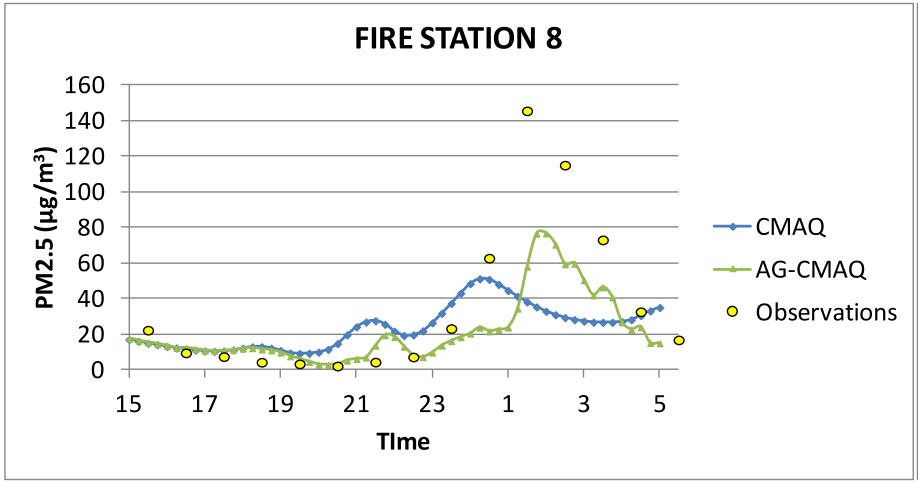


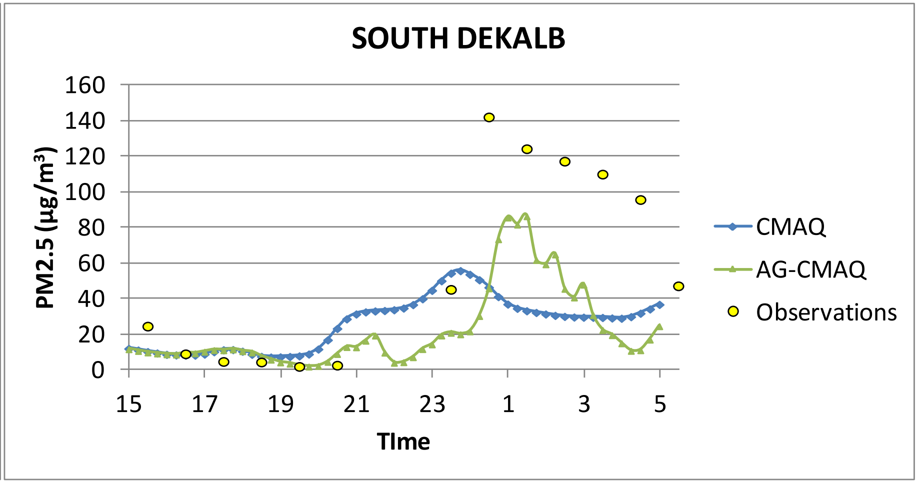
- CMAQ-SMOKE-WRF modeling system
- BlueSky modeling framework
- Fire Emissions Production Simulator

Adaptive Grid Evaluation in CMAQ









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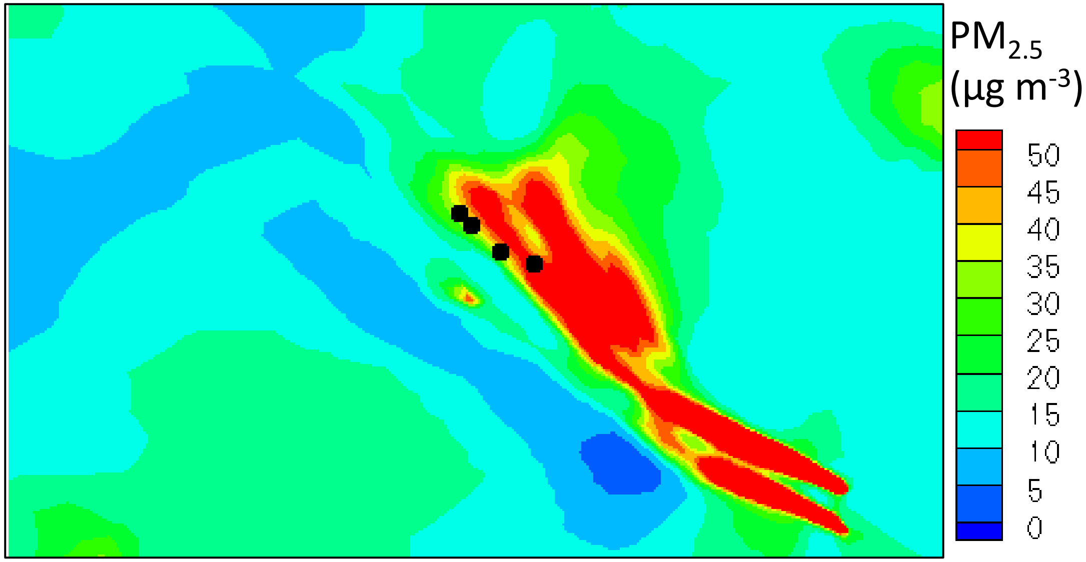
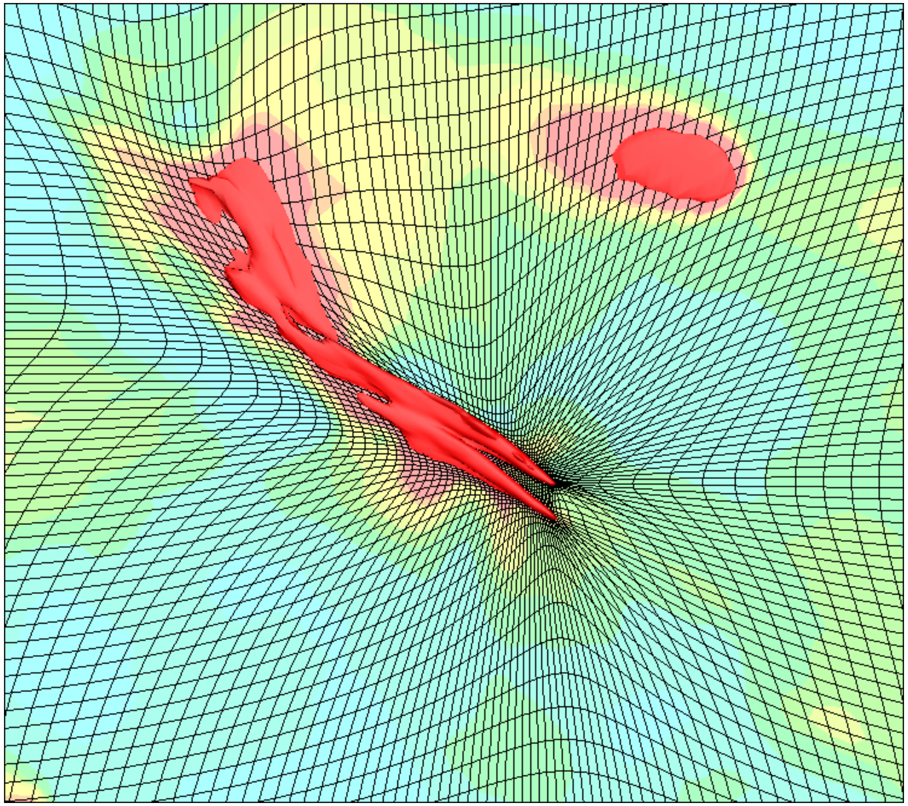
Adaptive Grid CMAQ Evaluation



Monitoring Site:	Mean Fractional Error		Peak $PM_{2.5}$ ($\mu g\ m^{-3}$)		
	Fixed Grid	*Adaptive Grid*	*Observed*	*Fixed Grid*	*Adaptive Grid*
Jeff St.	78%	58%	134	49	82
Conf. Av.	66%	58%	148	47	84
S. DeKalb	86%	79%	142	56	87
Fire St. 8	72%	65%	146	51	77

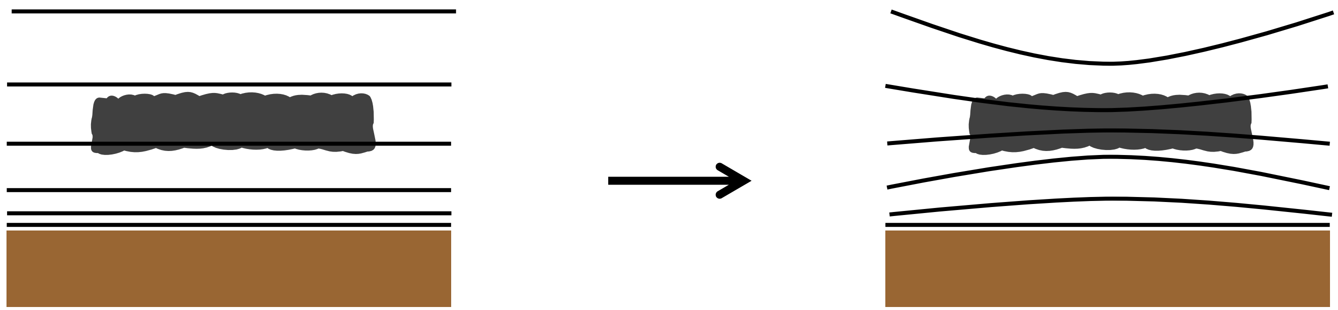
Observations from Adaptive Grid Evaluations

- Artificial diffusion is reduced.
- Predictions frequently better agree with monitoring site observations.
- Underprediction of air quality impacts is improved (but still significant).
- Adaptive grid simulations 35% slower than fixed grid.

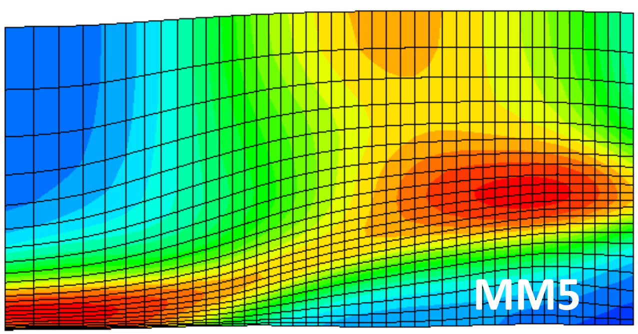


Future Work

- Implement adaptive grid algorithm into CMAQ 5.0
- Complete extension of adaptive grid into vertical grid structure



- Explore adaptive grid meteorological modeling driven by CMAQ-derived concentrations



THANK YOU!

Strategic Environmental Research and Development Program

Joint Fire Science Program

Georgia Department of Natural Resources, Environmental Protection Division

US Forest Service, Southern Research Station