

# Supplementary Material

## GPU-HADVPPM V1.0: high-efficient parallel GPU design of the Piecewise Parabolic Method (PPM) for horizontal advection in air quality model (CAMx V6.10)

Kai Cao<sup>1</sup>, Qizhong Wu<sup>1</sup>, Lingling Wang<sup>2</sup>, Nan Wang<sup>2</sup>, Huaqiong Cheng<sup>1</sup>, Xiao Tang<sup>3</sup>, Dongqing Li<sup>1</sup>, and Lanning Wang<sup>1</sup>

<sup>1</sup>College of Global Change and Earth System Science, Beijing Normal University, Beijing 100875, China

<sup>2</sup>Henan Ecological Environmental Monitoring Centre and Safety Center, Henan Key Laboratory of Environmental Monitoring Technology, Zhengzhou 450008, China

<sup>3</sup>State Key Laboratory of Atmospheric Boundary Layer Physics and Atmospheric Chemistry, Institute of Atmospheric Physics, Chinese Academy of Science, Beijing 100029, China

Correspondence to: Qizhong Wu ([wqizhong@bnu.edu.cn](mailto:wqizhong@bnu.edu.cn)); Lingling Wang([928216422@qq.com](mailto:928216422@qq.com)); Lanning Wang ([wangln@bnu.edu.cn](mailto:wangln@bnu.edu.cn))

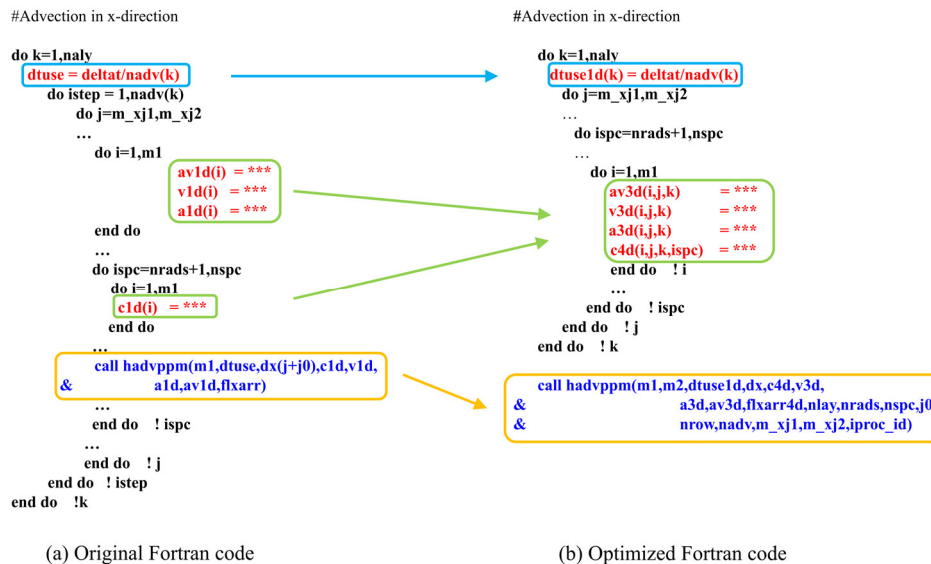
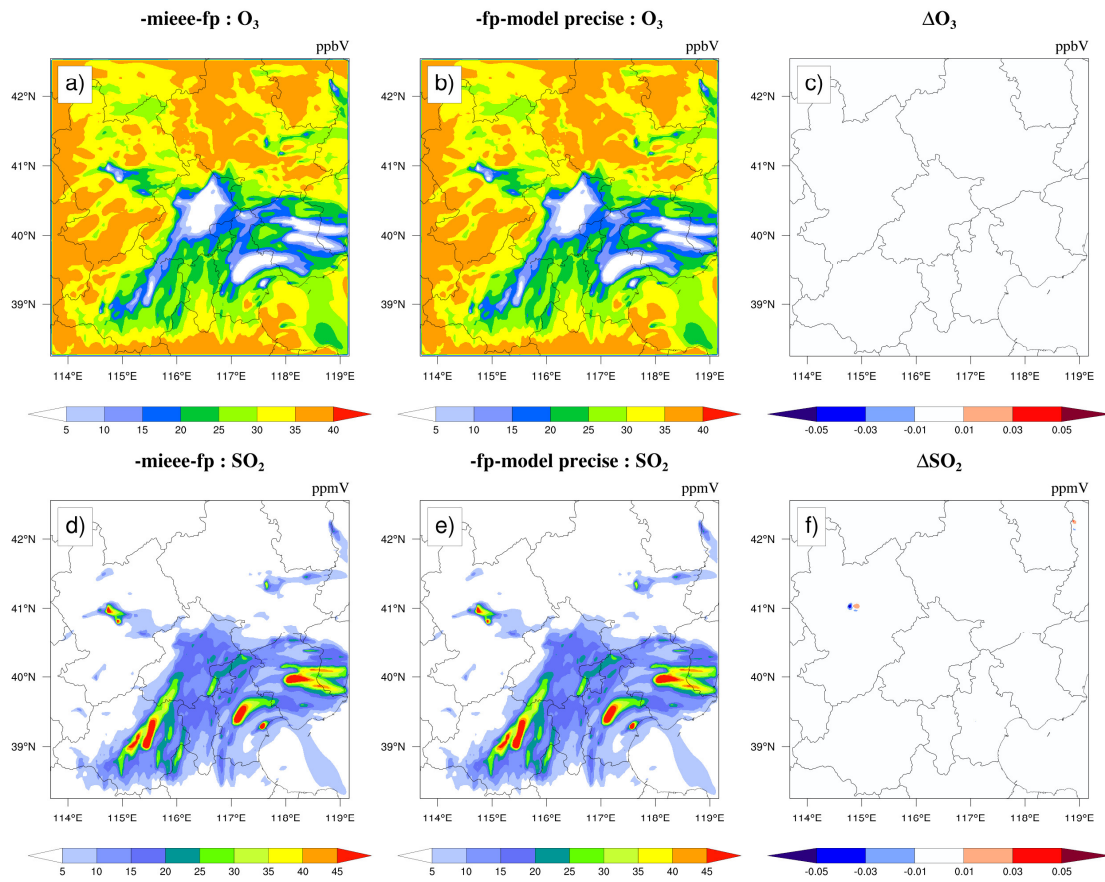


Figure S1. An example of xyadvec Fortran program optimization. (a) and (b) represent original code and optimized code, respectively.



23

24 Figure S2. The absolute errors (AEs) of the simulation results between the *-fp model*  
 25 *precise* and *-miecee-fp* compile flags.

26

27 Table S1. Variable names input into the HADVPPM program and their specific  
 28 meanings.

29

Name	Specific Meanings (Unit)
<i>nn</i>	Number of cells
<i>dt</i>	Time step (s)
<i>dx</i>	Length of cell (m)
<i>con</i>	Concentration vector ( $\mu\text{mol} \cdot \text{m}^{-3}$ )

---

<i>vel</i>	Wind speed vector ( $m \cdot s^{-1}$ )
<i>area</i>	Cell area adjustment vector ( $m^{-2}$ )
<i>areav</i>	Interfacial area adjustment vector ( $m^2$ )

---

30

31 Table S2. The physical and chemical numerical methods selected during CAMx  
 32 integration

33

---

<b>Process</b>	<b>Numerical Methods</b>
Horizontal advection	PPM (Colella and Woodward, 1984)
Vertical diffusion	K-theory 1 <sup>st</sup> order closure
Aqueous-phase oxidation	Regional Acid Deposition Model (RADM-AQ, (Chang et al., 1987))
Inorganic aerosol thermodynamic partitioning	ISORROPIA (Nenes et al., 1999)
Gas-Phase Chemistry	Carbon Bond 2005 (Yarwood et al., 2005) EBI solver (Hertel et al., 1993)
Dry deposition	Resistance model for gases (Zhang et al., 2003) and aerosols (Zhang et al., 2001)
Wet deposition	Scavenging model for gases and aerosols (Seinfeld et al., 1998)

---

34 **Reference**

35

36 Chang, J. S., Brost, R. A., Isaksen, I. S. A., Madronich, S., Middleton, P., Stockwell, W.  
 37 R., and Walcek, C. J.: A three-dimensional Eulerian acid deposition model:  
 38 Physical concepts and formulation, *Journal of Geophysical Research:*  
 39 *Atmospheres*, 92, 14681-14700, <https://doi.org/10.1029/JD092iD12p14681>, 1987.  
 40 Colella, P. and Woodward, P. R.: The Piecewise Parabolic Method (PPM) for gas-  
 41 dynamical simulations, *Journal of Computational Physics*, 54, 174-201,  
 42 [https://doi.org/10.1016/0021-9991\(84\)90143-8](https://doi.org/10.1016/0021-9991(84)90143-8), 1984.  
 43 Hertel, O., Berkowicz, R., Christensen, J., and Hov, Ø.: Test of two numerical schemes  
 44 for use in atmospheric transport-chemistry models, *Atmospheric Environment*.

45 Part A. General Topics, 27, 2591-2611, <https://doi.org/10.1016/0960->  
46 1686(93)90032-T, 1993.

47 Nenes, A., Pandis, S. N., and Pilinis, C.: Continued development and testing of a new  
48 thermodynamic aerosol module for urban and regional air quality models,  
49 Atmospheric Environment, 33, 1553-1560, <https://doi.org/10.1016/S1352->  
50 2310(98)00352-5, 1999.

51 Seinfeld, J. H., Pandis, S. N., and Noone, K. J. J. P. T.: Atmospheric Chemistry and  
52 Physics: From Air Pollution to Climate Change, 51, 88-90, 1998.

53 Yarwood, G., Rao, S., Yocke, M., and Whitten, G.: Updates to the carbon bond chemical  
54 mechanism: CB05 final report to the US EPA, RT-0400675, 2005.

55 Zhang, L., Brook, J. R., and Vet, R.: A revised parameterization for gaseous dry  
56 deposition in air-quality models, Atmos. Chem. Phys., 3, 2067-2082, 10.5194/acp-  
57 3-2067-2003, 2003.

58 Zhang, L., Gong, S., Padro, J., and Barrie, L.: A size-segregated particle dry deposition  
59 scheme for an atmospheric aerosol module, Atmospheric Environment, 35, 549-  
60 560, [https://doi.org/10.1016/S1352-2310\(00\)00326-5](https://doi.org/10.1016/S1352-2310(00)00326-5), 2001.

61  
62