



*Supplement of*

## **GPU-HADVPPM V1.0: a high-efficiency parallel GPU design of the piecewise parabolic method (PPM) for horizontal advection in an air quality model (CAMx V6.10)**

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# Supplementary Material

```

#Advection in x-direction
do k=1,nalv
  dtuse = deltat/nadv(k)
  do istep = 1,nadv(k)
    do j=m_xj1,m_xj2
      ...
      do i=1,m1
        av1d(i) = ***
        v1d(i) = ***
        a1d(i) = ***
      end do
      ...
      do ispc=nrads+1,nspe
        do i=1,m1
          c1d(i) = ***
        end do
        ...
        call hadvppm(m1,dtuse,dx(j+j0),c1d,v1d,
          & a1d,av1d,flxarr)
        ...
      end do ! ispc
    end do ! j
  end do ! istep
end do ! k

```

(a) Original Fortran code

```

#Advection in x-direction
do k=1,nalv
  dtuse1d(k) = deltat/nadv(k)
  do j=m_xj1,m_xj2
    ...
    do ispc=nrads+1,nspe
      ...
      do i=1,m1
        av3d(i,j,k) = ***
        v3d(i,j,k) = ***
        a3d(i,j,k) = ***
        c4d(i,j,k,ispc) = ***
      end do ! i
    end do ! ispc
  end do ! j
end do ! k

```

(b) Optimized Fortran code

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

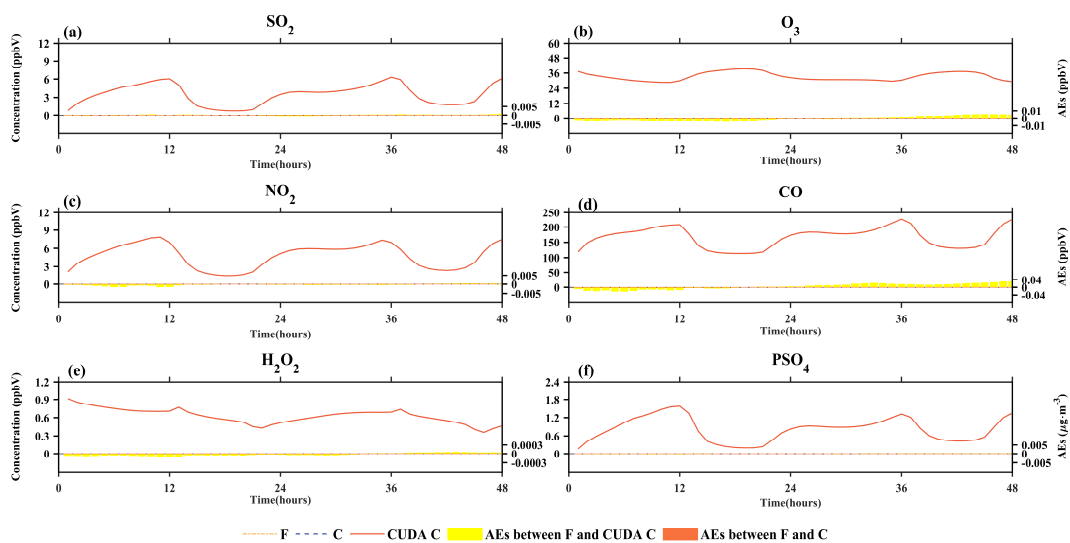


Figure S2. Time series and AEs of SO<sub>2</sub>, O<sub>3</sub>, NO<sub>2</sub>, CO, H<sub>2</sub>O<sub>2</sub>, and PSO<sub>4</sub> outputted by CAMx model for Fortran, standard C, and CUDA C versions.

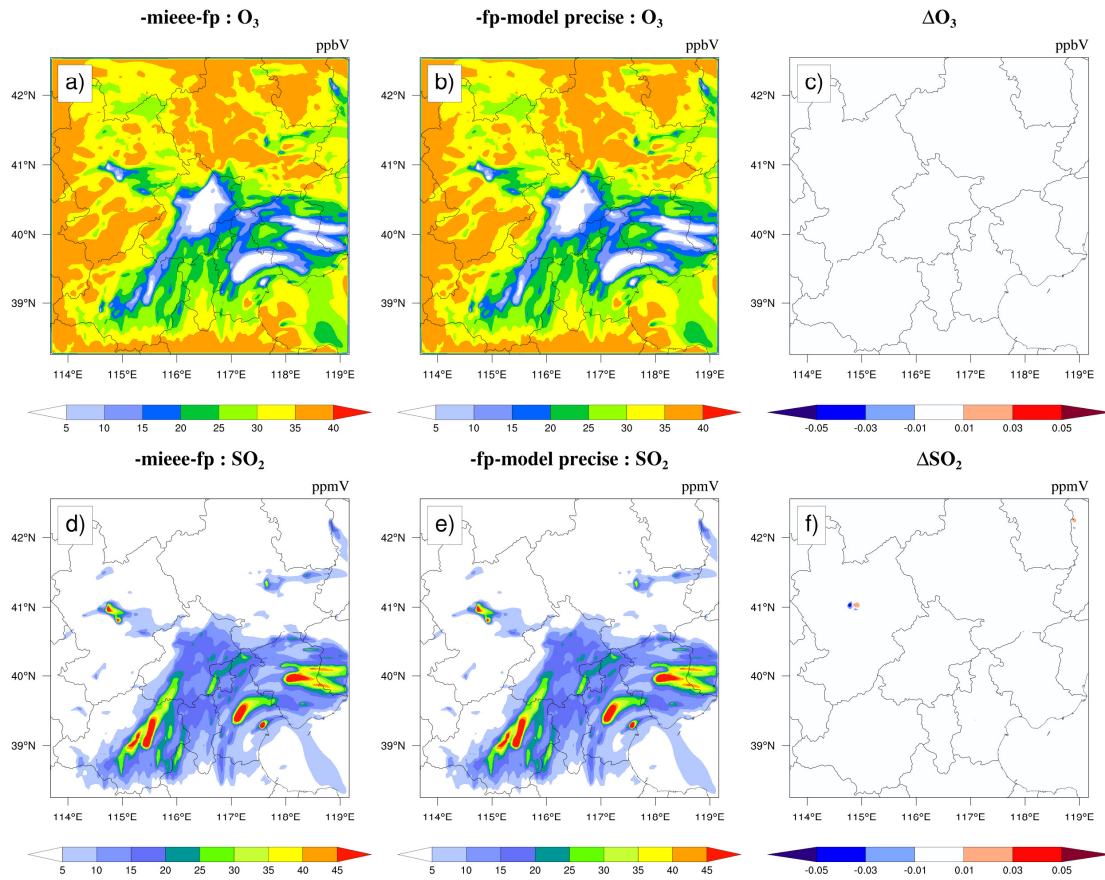


Figure S3. The absolute errors (AEs) of the simulation results between the *-fp model precise* and *-miecee-fp* compile flags.

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

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 ( $\text{m} \cdot \text{s}^{-1}$ )

<i>area</i>	Cell area adjustment vector ( $m^{-2}$ )
<i>areav</i>	Interfacial area adjustment vector ( $m^2$ )

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

<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)

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