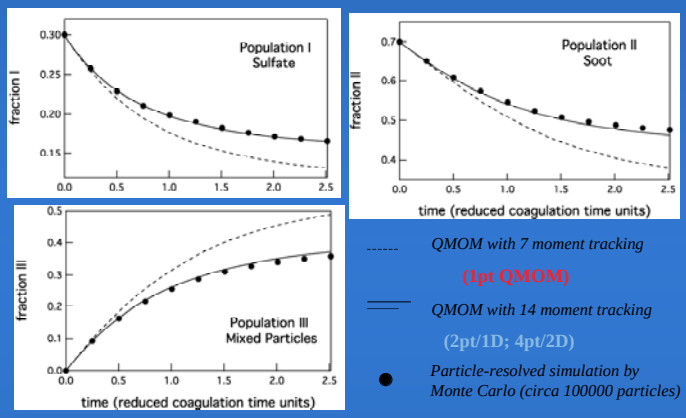
SIMULATING AEROSOL MIXING STATE USING THE QUADRATURE METHOD OF MOMENTS (QMOM)

Our goal is to develop and test a QMOM aerosol dynamics module suitable for use in climate models

• In the method of moments only the moments of the particle size distribution are tracked in time, which makes the method highly efficient. Quadrature, with Q-points, selected to reproduce the tracked moments, are used to close evolution equations for the moments and also to approximate aerosol physical and optical properties in terms of the moments.

Benchmarking QMOM accuracy against particle-resolved (P-R) simulation

• Here we simulate the mixing states of soot and sulfate particles undergoing coagulation. This important "aging" mechanism determines aerosol optical properties and cloud condensation nuclei (CCN) concentrations in the atmosphere.



QMOM simulations on laptop in under 1 second

Figure 2. Evolution of particle number fractions: soot + sulfate -> mixed particles. Comparing results using two QMOM schemes. Circles :results from P-R simulation. Dashed curves: results from 7 moment tracking, equivalent to tracking 1 quadrature point for each mode. Solid curves: results from 14 moment tracking, including tracking the covariance matrix for the mixed mode. Equivalent to tracking 2 quadrature points for each of the initial modes and 4 equal-weight quadrature points for the mixed mode.

Current status of QMOM aerosol module development

• The 1 Q-point/mode scheme (dashed curves in Fig. 2) has been successfully implemented for tracking of particle number and mass in the NASA GISS ModelE [Bauer et al. ACPD, 8, 9931 (2008)]. Efforts are underway to implement the more accurate scheme of Fig. 2., which tracks through 2nd-order moments. This higher level of accuracy should be sufficient given the rapid convergence to P-R simulation results with increasing moment order seen in Fig.3.

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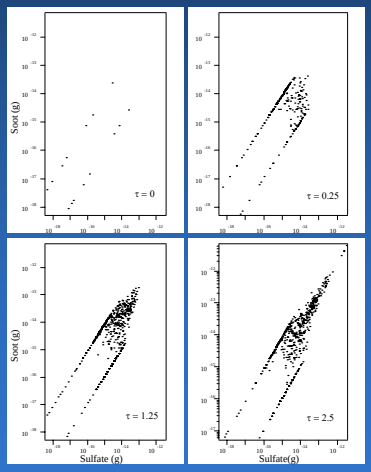

Figure 1. Sampled particles from P-R simulation. Initially two particle populations are present. Over time (reduced units) these mix, grow to CCN size and become internally mixed (as seen in the approaching constant composition of the largest particles, which have undergone the largest number of coagulation events

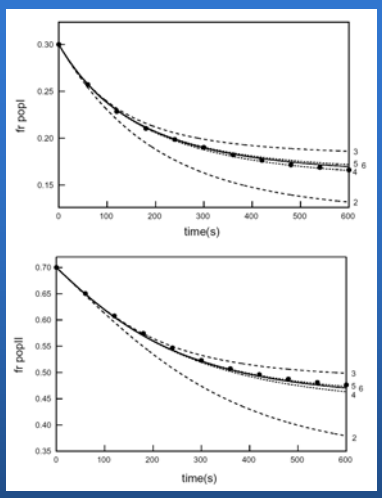

Figure 3. Comparing different quadrature schemes. Figures show the decay of initial populations I and II as the mixed population forms. Circles - results from P-R simulation. Curves - results obtained on tracking different numbers of moments (the number of tracked moments is indicated to the right of each curve). Gauss (Gauss-Radau) quadratures employ even (odd) numbers of moments and yield nested lower (upper) bounds..