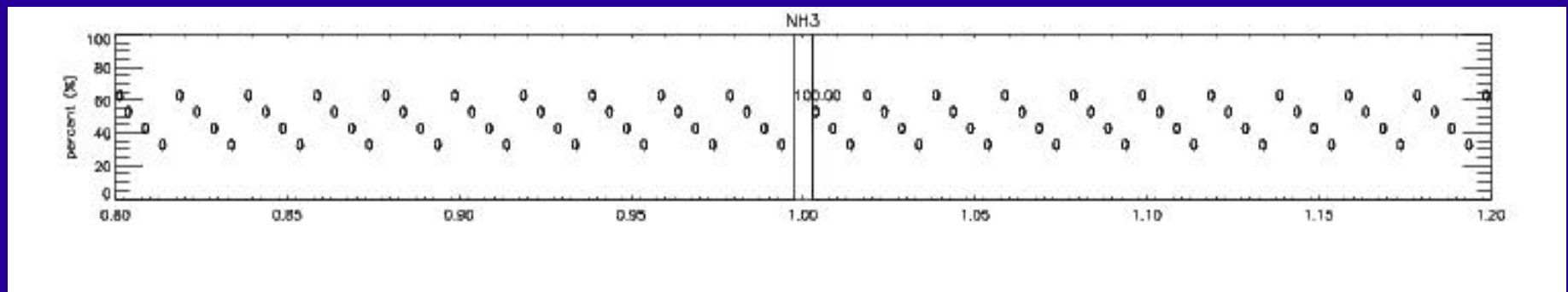


ISORROPIA numerical noise

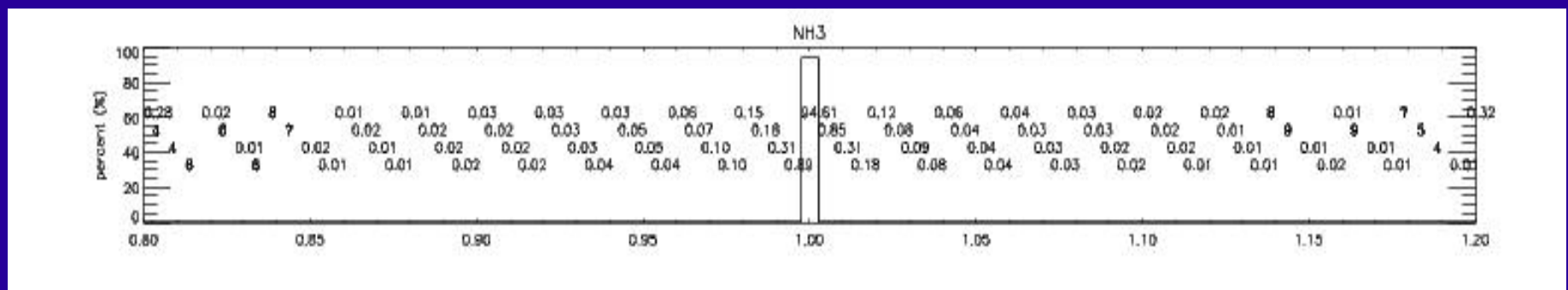
- ISORROPIA = aerosol thermodynamics. Equilibrium code
 - Partitions nitrate (HNO_3 and NIT) and ammonia (NH_3 and NH_4) between the gas and aerosol phases.
 - Inputs are temperature and RH.
- New benchmarking procedure (more frequent 1MBs) indicated that the ISORROPIA introduces numerical noise into the output
- Slight discrepancies seen in the G-C output
 - Especially for 1MBs that should have had identical results

ISORROPIA numerical noise

Frequency distribution histogram for NH₃
Comparing two 7-day simulations (ISORROPIA on vs. ISORROPIA off)



Frequency distribution histogram for NH₃
Comparing two 20-day simulations (ISORROPIA on vs. ISORROPIA off)



ISORROPIA numerical noise

- HNO₃, NIT, NH₃, NH₄ are affected
- Noise is seen in runs of ~2 weeks or longer
- Appears to be caused by compiler optimization
- Using “safe” optimization flags didn't help
- ISORROPIA is “spaghetti code”; Hard to find bugs
- I brought this to the attention of the Nenes group at GT. Shannon Capps was looking into this.

ISORROPIA numerical noise

- For most GC users:
 - You can pretty much ignore this. The noise is not large enough to influence the results of a long simulation.
- For more advanced code developers:
 - If you are debugging a new feature, we recommend that you comment out the call to ISORROPIA in module `chemistry_mod.F`.
 - Especially if you are expect to see identical results (i.e. if you are restructuring code but not changing any science)