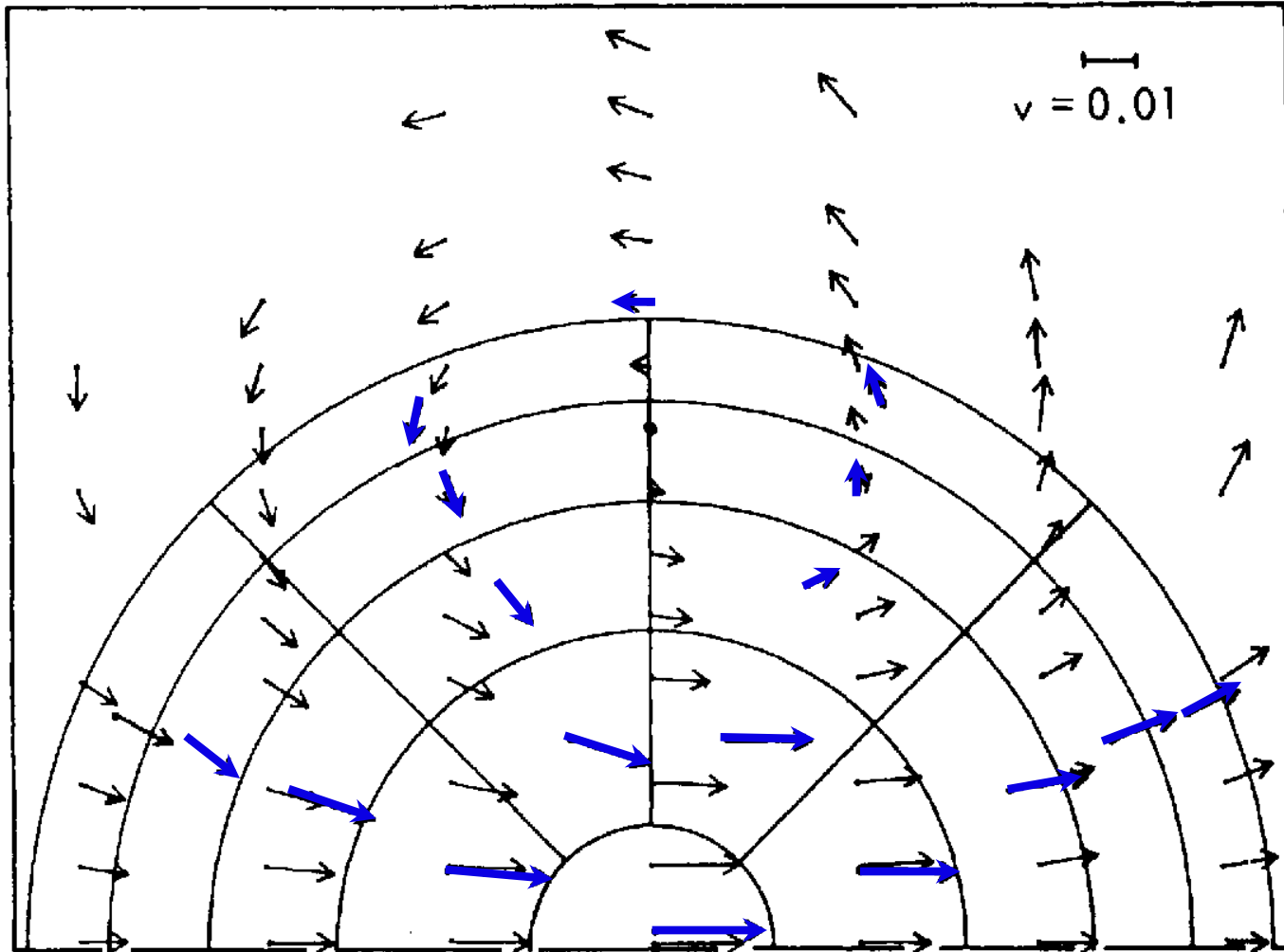


5.2

Lecture 5.2: Key points, and what next?

- * Emergence of organized flow in a randomized (thermal) gas
- * Existence of scale invariance in atmospheric observations
- * Correlations among scaling exponents
- * Overpopulation of high-speed molecules in air
- * Thermodynamic formulation of scale invariance

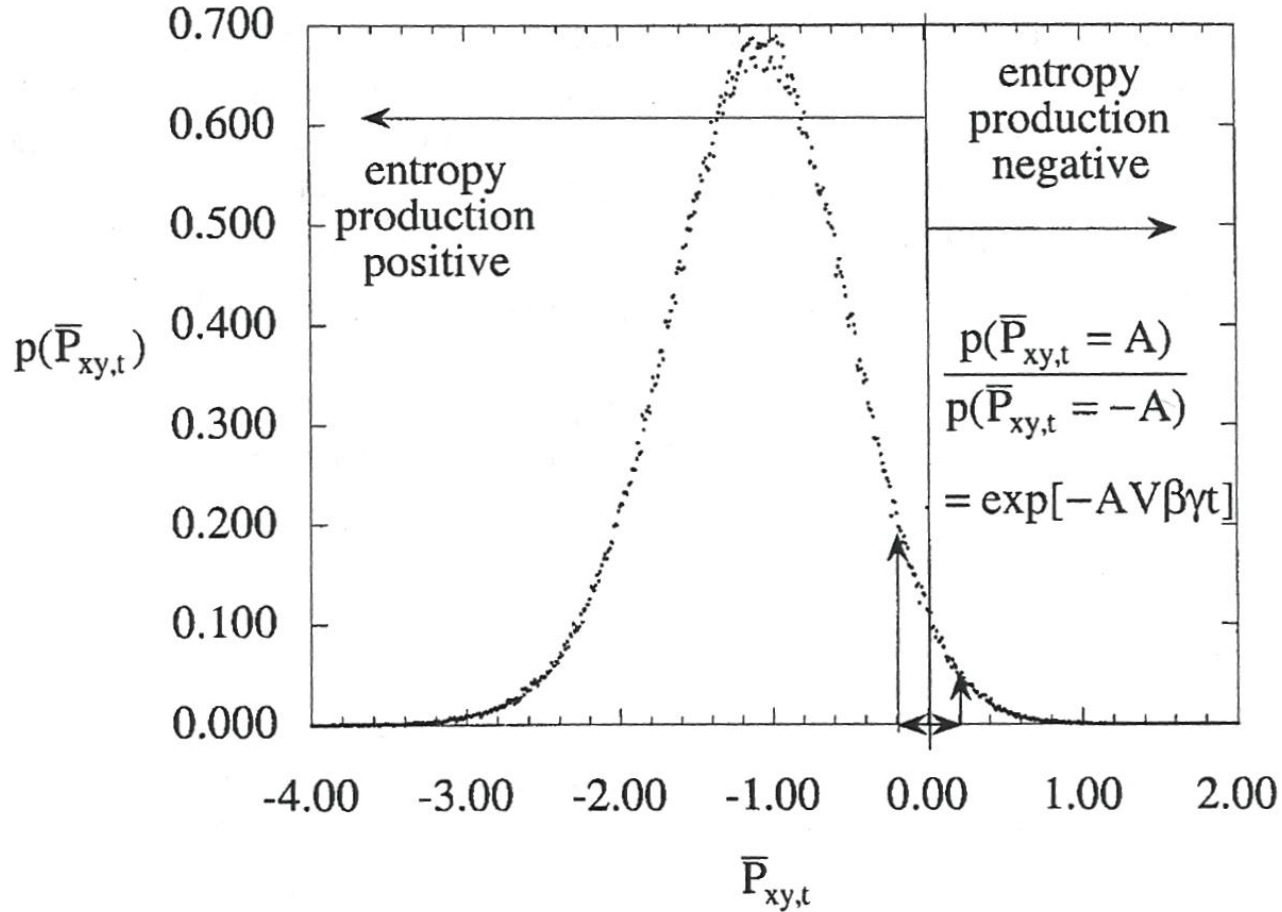
Alder & Wainwright (1970): **molecular dynamics** simulation of a flux applied to an equilibrated Maxwellian population results in the emergence of vortices on scales of 10^{-12} seconds & 10^{-8} metres.



Evans & Searles (2002), *Adv. Phys.*, 51,1529-1585. The minority high speed molecules, produce organization ('flow') while the average majority produce dissipation ('temperature').

The Fluctuation Theorem

$t = 0.1, \gamma = 0.5$



Emergence of organized flow in a randomized gas

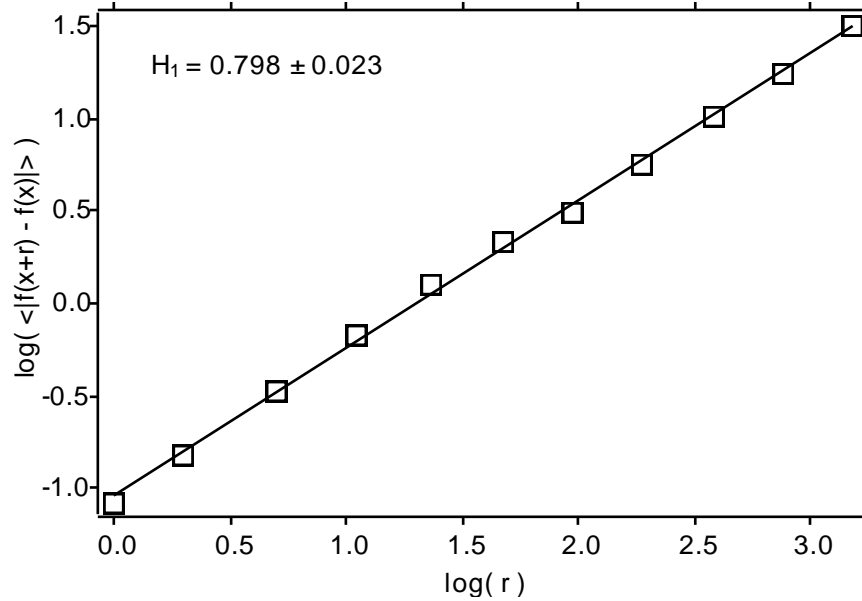
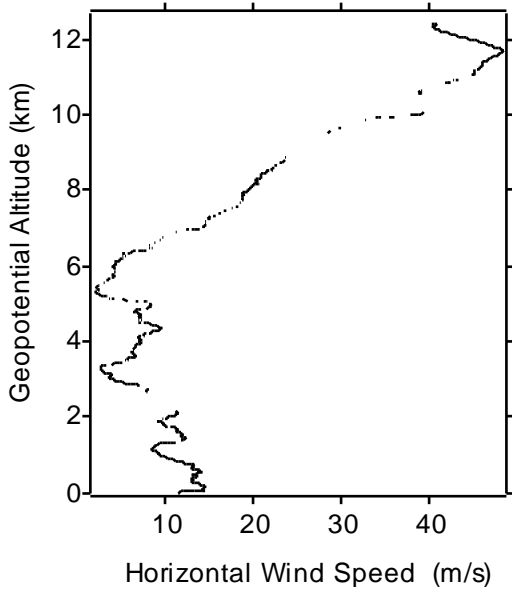
- * Production of vorticity at scale of molecular mean free path.
- * No local thermodynamic equilibrium, no isotropic diffusion.
- * Fastest molecules cause flow, average ones define temperature.
- * Opposite of conventional meteorological decomposition into an organized mean and dissipative eddies.
- * Embodies the three essential elements of natural selection.

What to do about it?

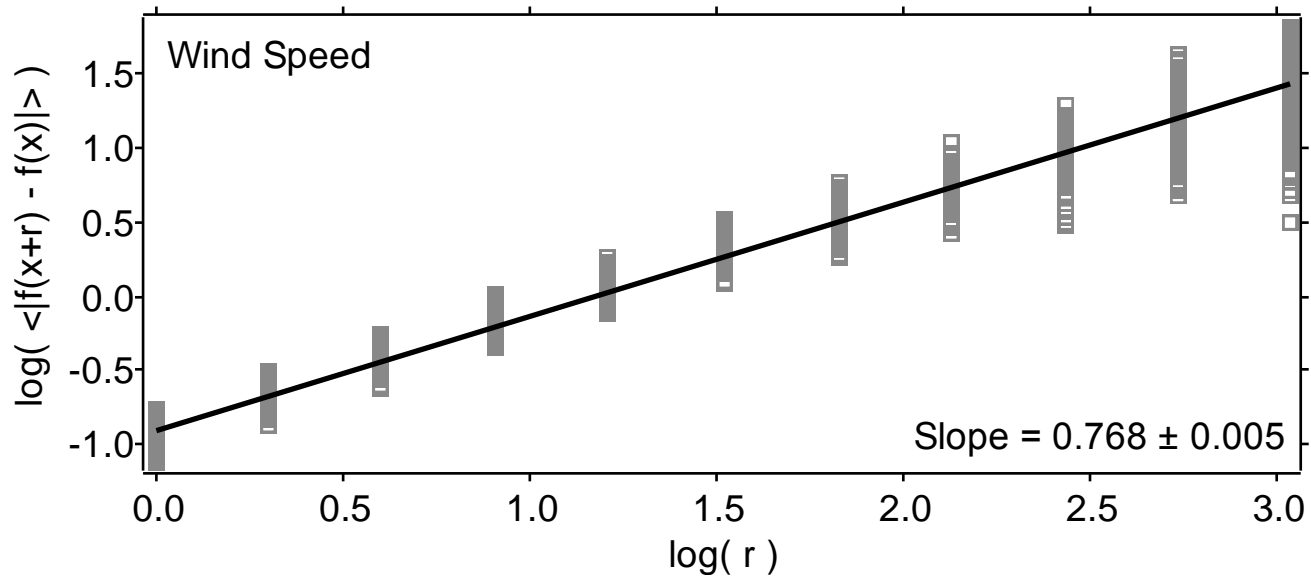
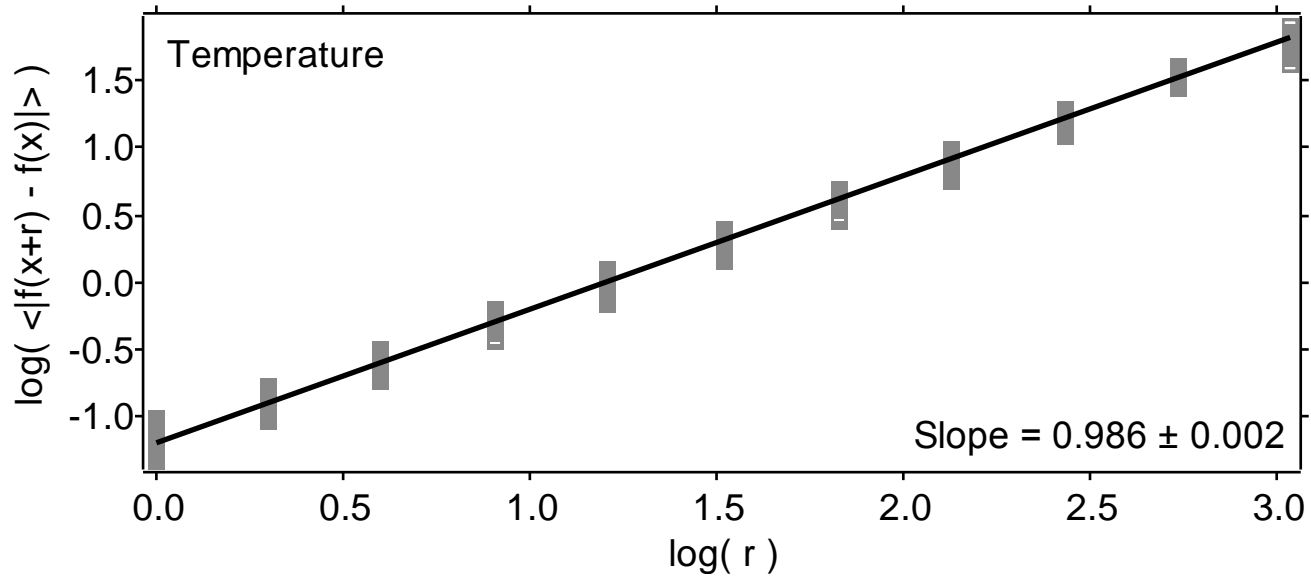
- * Molecular dynamics simulation of lower stratospheric air.
- * Experimental tests of better atmospheric observations.
- * Develop better model formulations, dynamically and radiatively.

Dropsonde from NOAA G4: (15°N, 166°W), 20040304

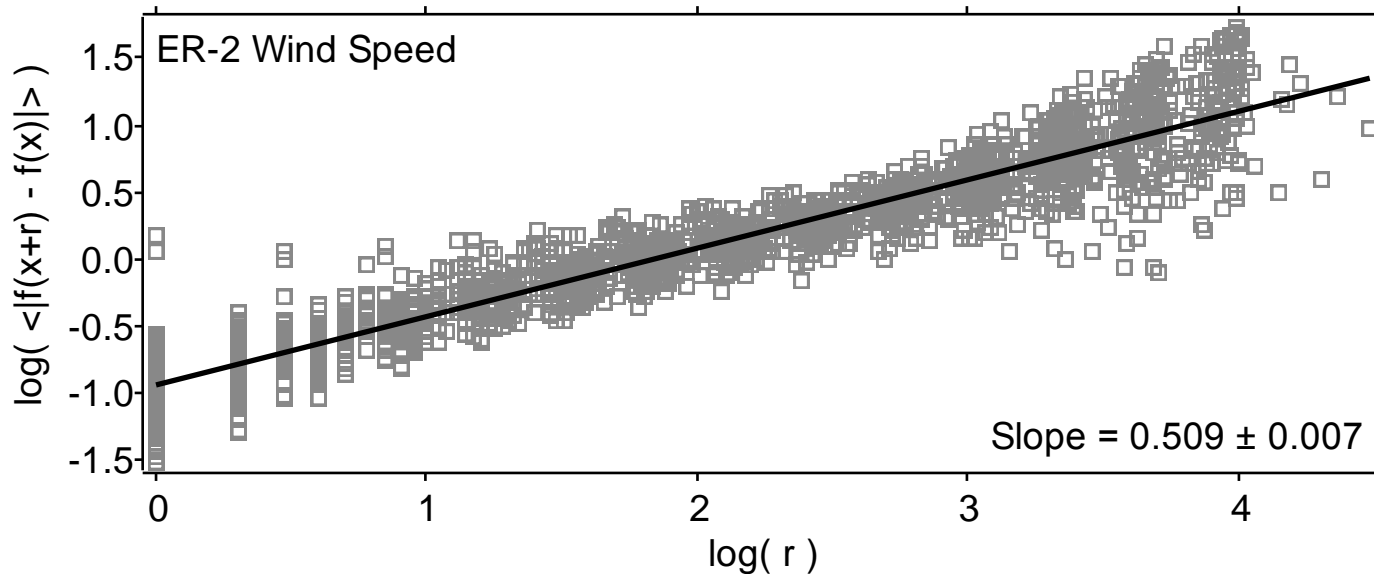
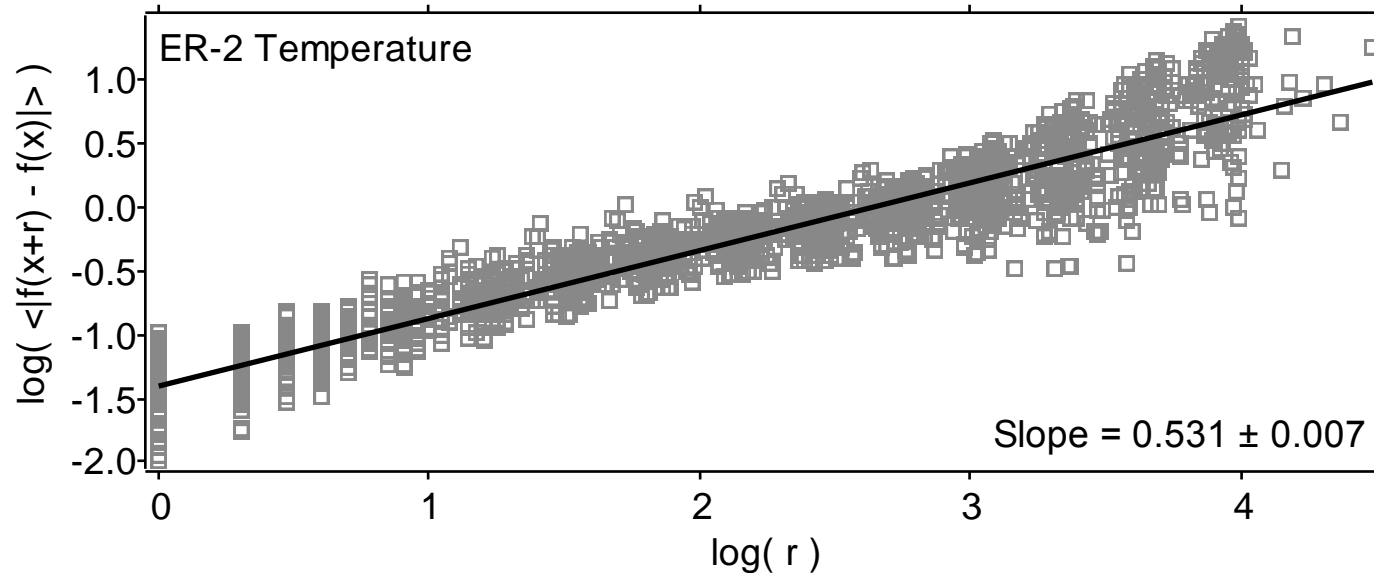
Wind speed & its H scaling exponent



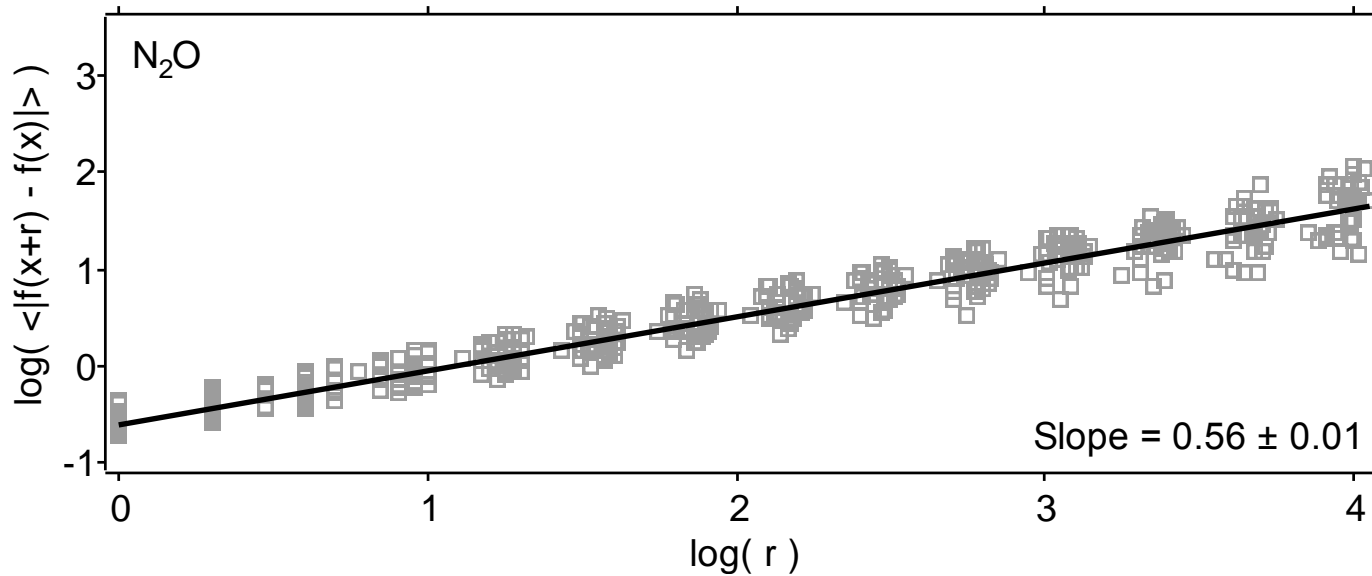
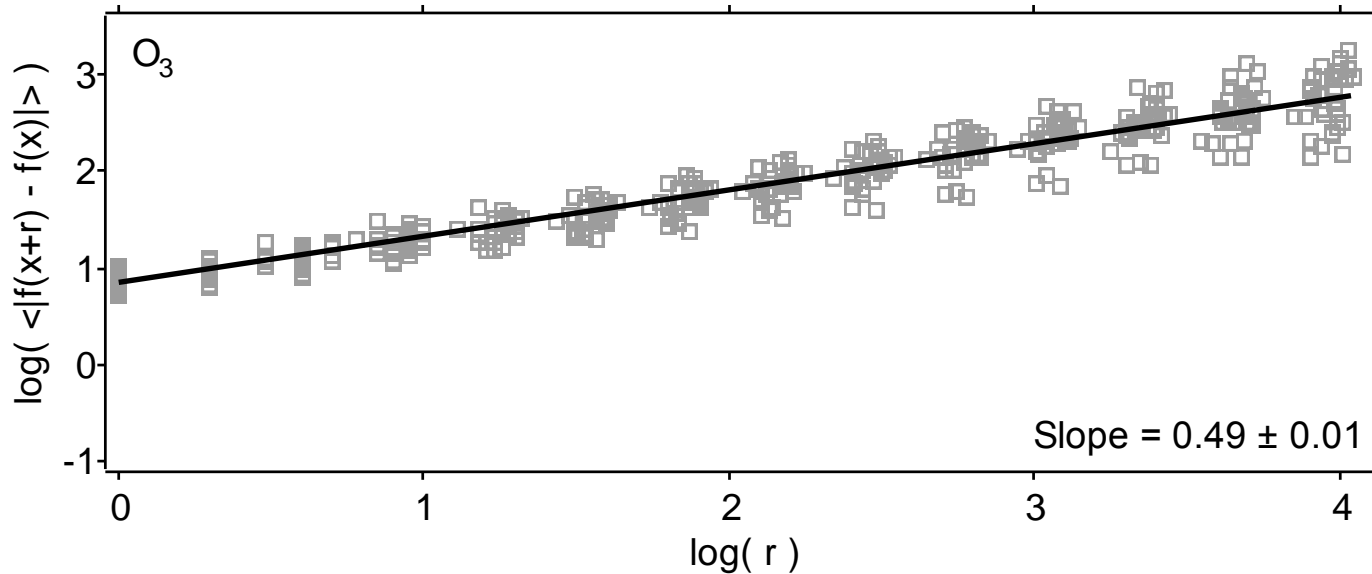
All 261 dropsondes, 20040229 - 20040315, 10° - 46° N, 140° - 172° W



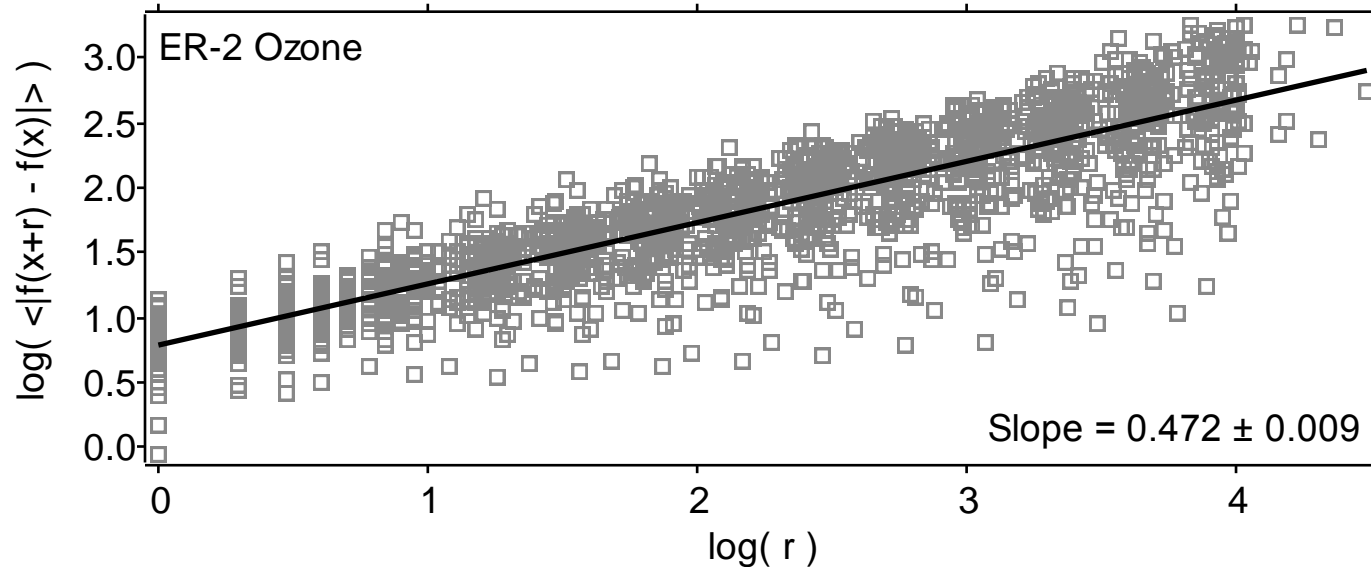
All ER-2 flight segments, 1987 - 2000, 90°N -72°S °



All ER-2 ozone & nitrous oxide, 59°N-70°S, heavy SH weighting

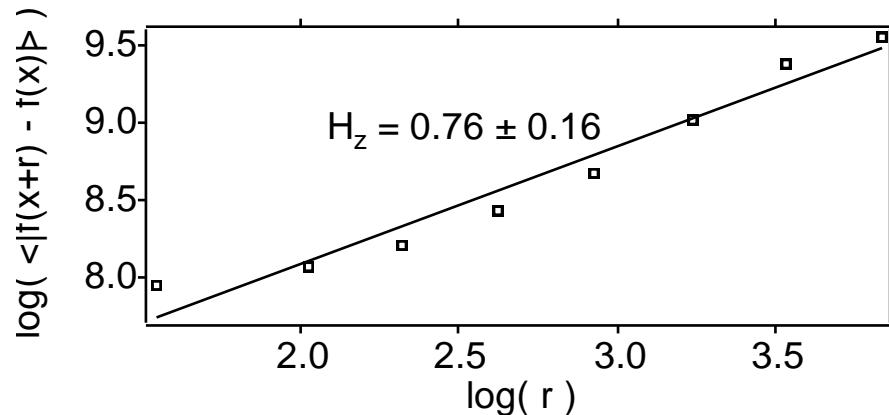
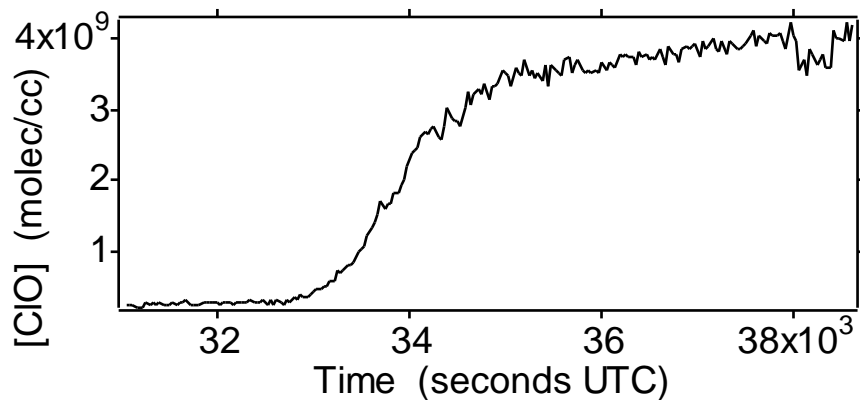


All ER-2 'horizontal' segments >2000 s, 1987-2000

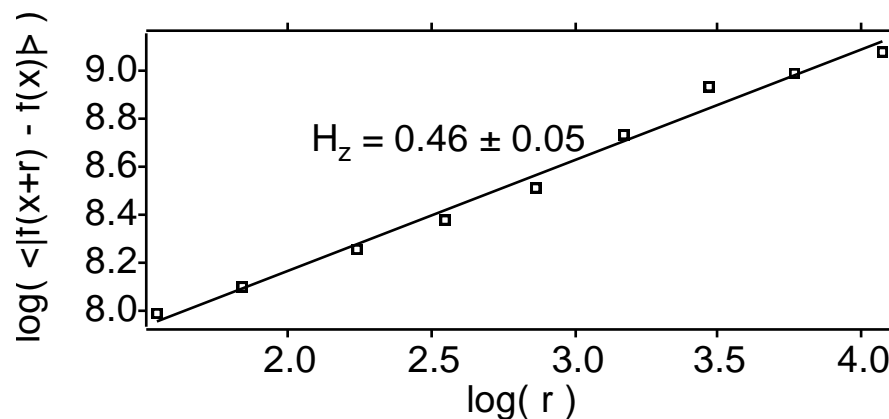
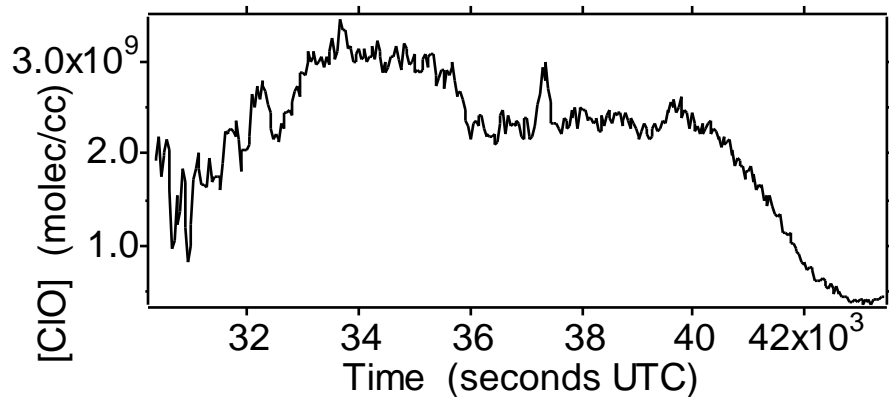


O_3 sink in polar vortex: $H < 5/9$

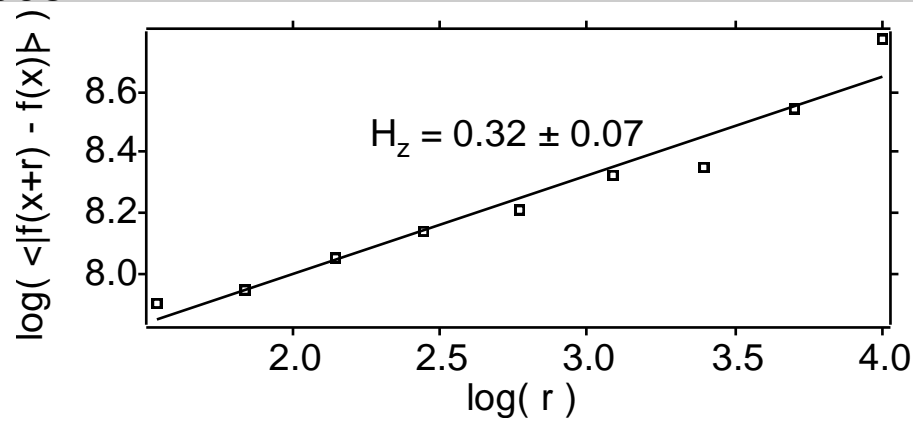
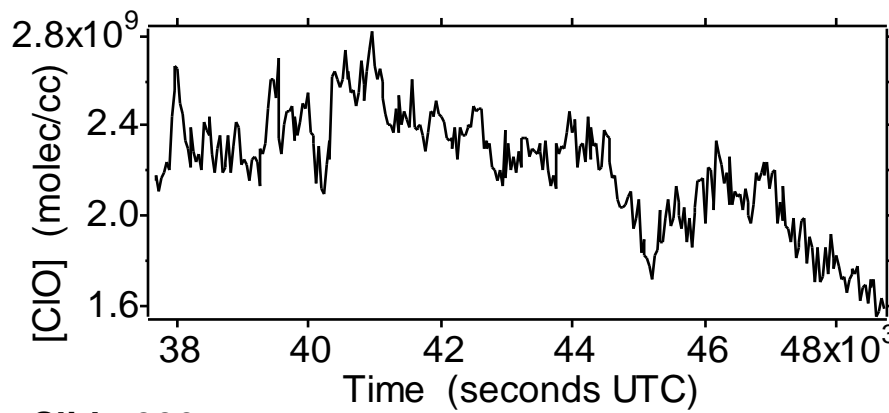
20000123



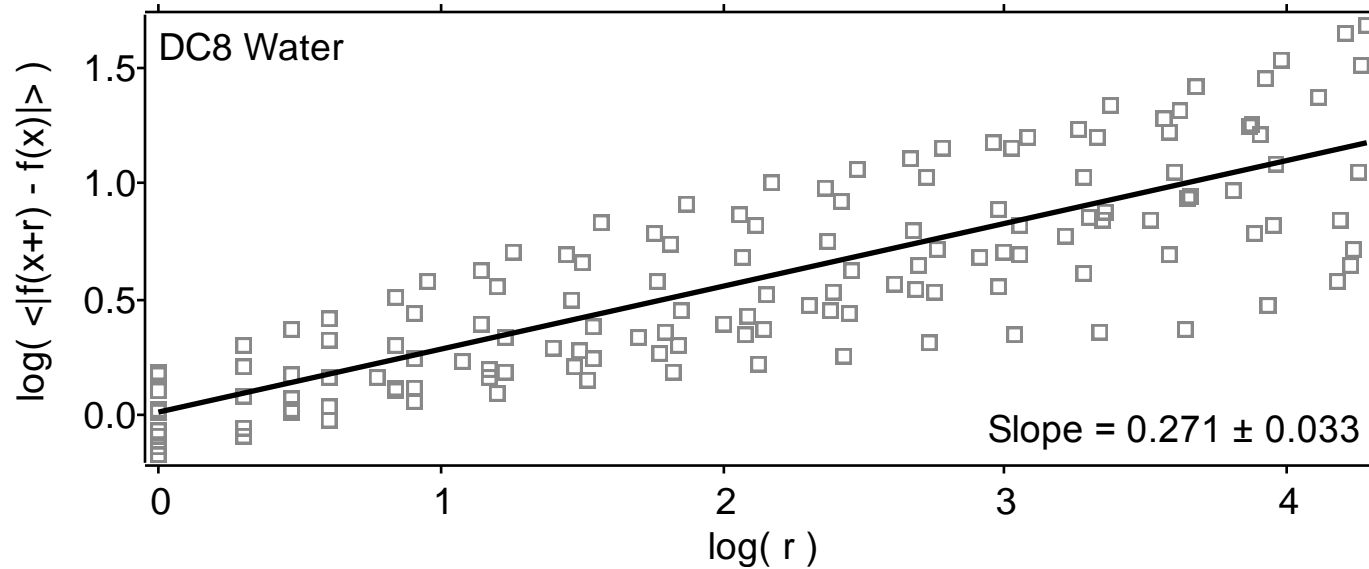
20000226



20000312

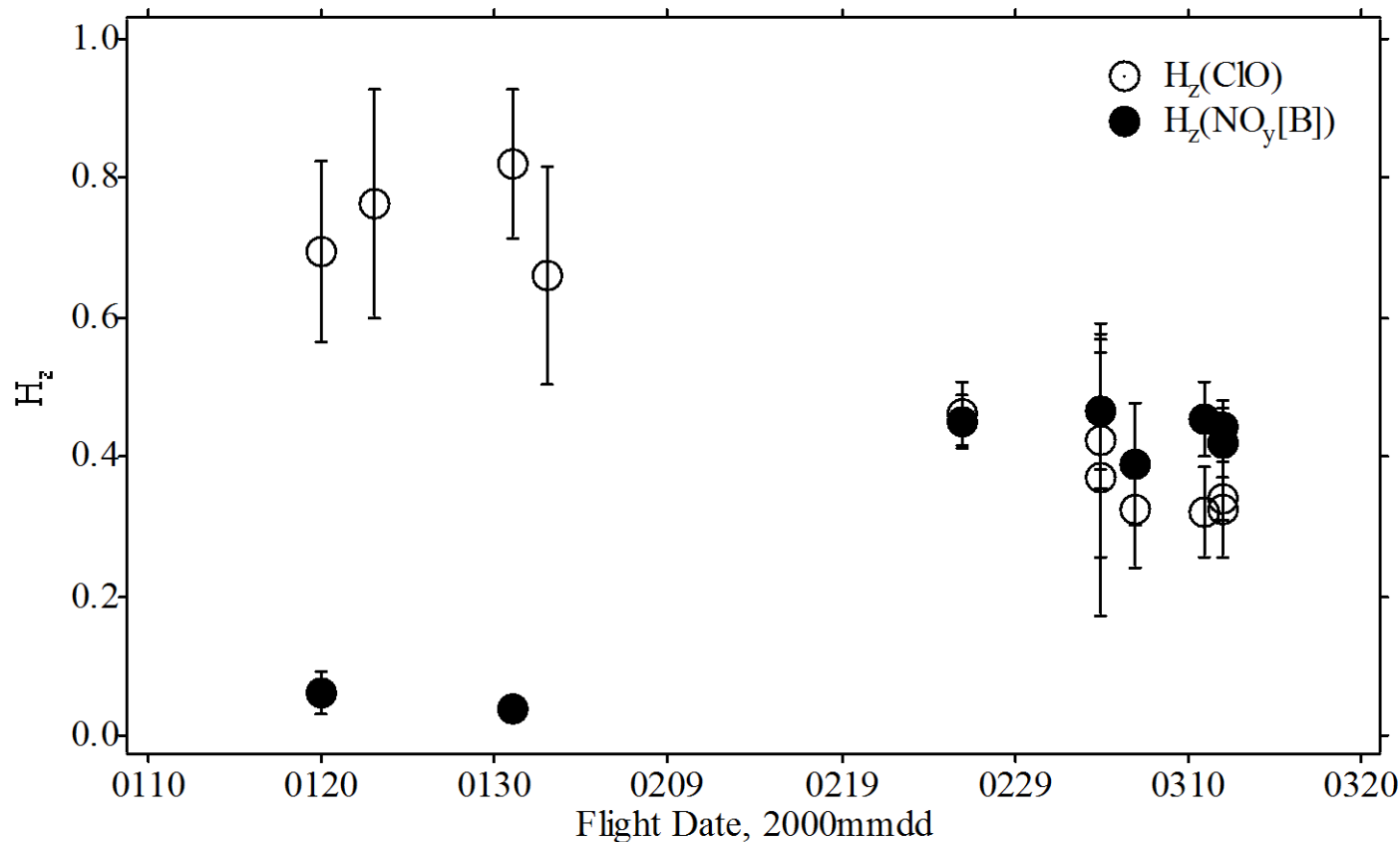


All DC-8 total water, 'horizontal', 44°S - 90°S, Aug-Sep 1987



$H < 5/9$ indicates a sink is operative - gravitational settling of ice

ER-2 scaling exponents for ClO and NO_y, Arctic vortex, January - March 2000. An early ClO source & NO_y sink from PSCs evolve to a sink and to a passive scalar (tracer) respectively.



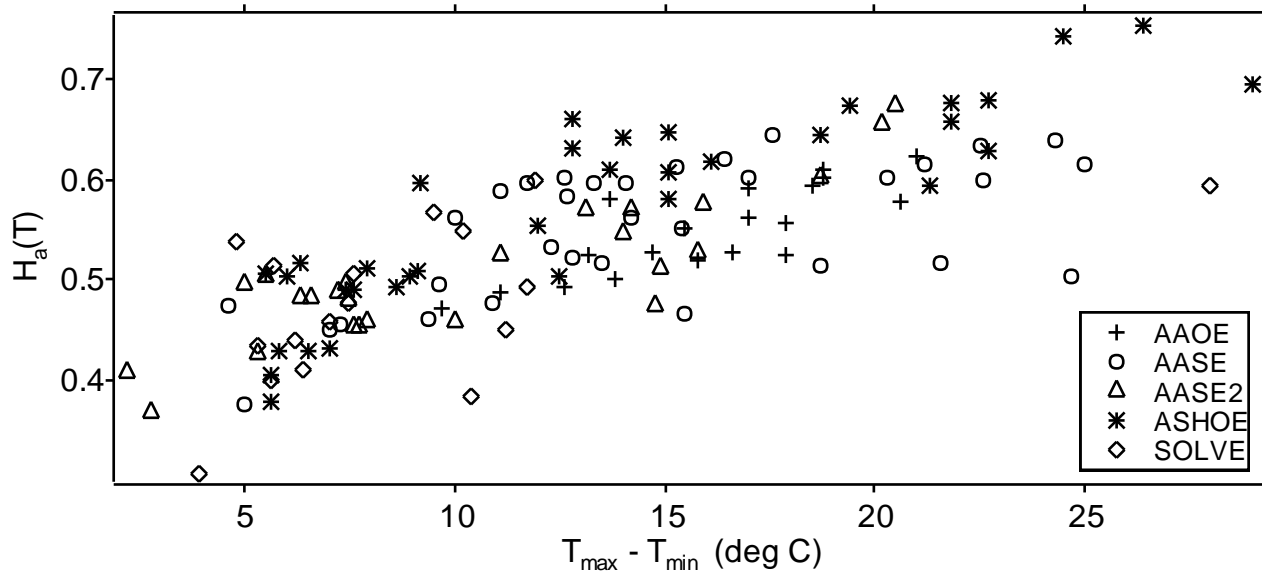
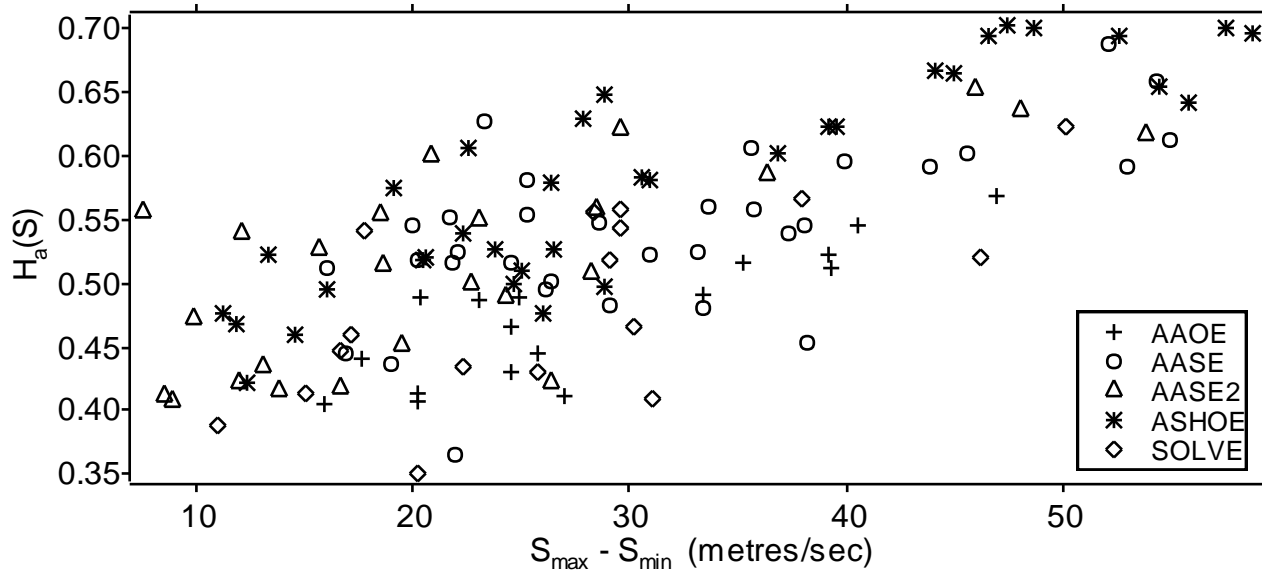
Existence of scale invariance in atmospheric observations

- * Ratio of $H_{\text{horiz}}/H_{\text{vert}}$ predicted to be 1 for Kolmogorov, 0 for 2D turbulence, $1/3$ for linear gravity wave theory and $5/9$ for generalized scale invariance.
- * Vertical scaling different than horizontal.
- * No stable layers.
- * T scales differently than other variables.
- * Variances do not converge.
- * $H(\text{chemical}) = 0.56$ for tracer, >0.56 for source, <0.56 for sink. True for N_2O , O_3 , ClO , NO_y and total water.

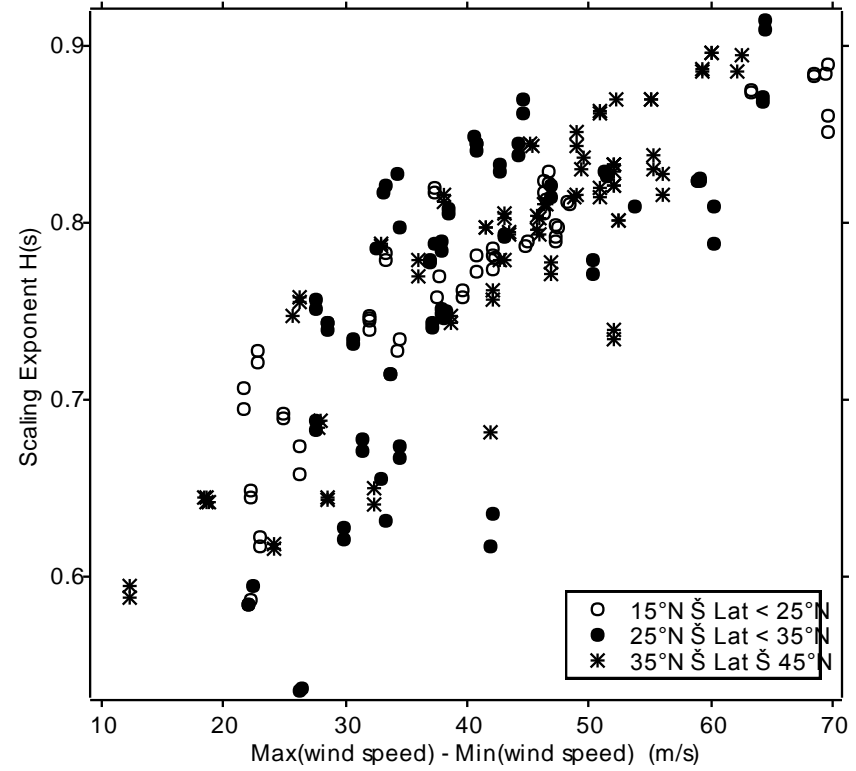
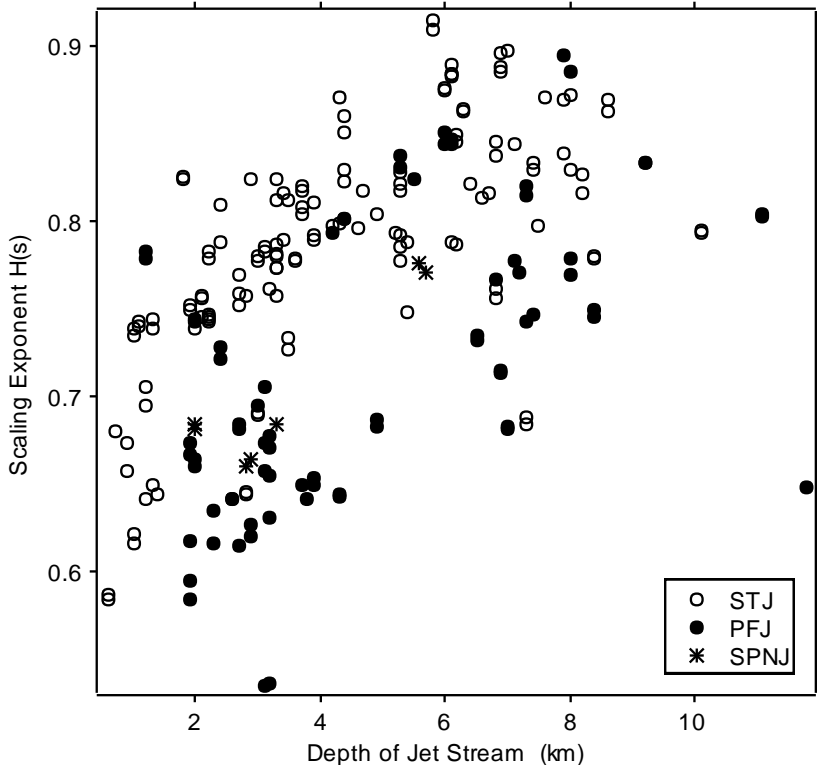
What to do about it?

- * If possible, get better observations in true horizontal and vertical directions.
- * Test source/sink results with more species, and see if results are consistent with the thermodynamic formulation of scale invariance.
- * Systematic testing of models - effective on all scales.

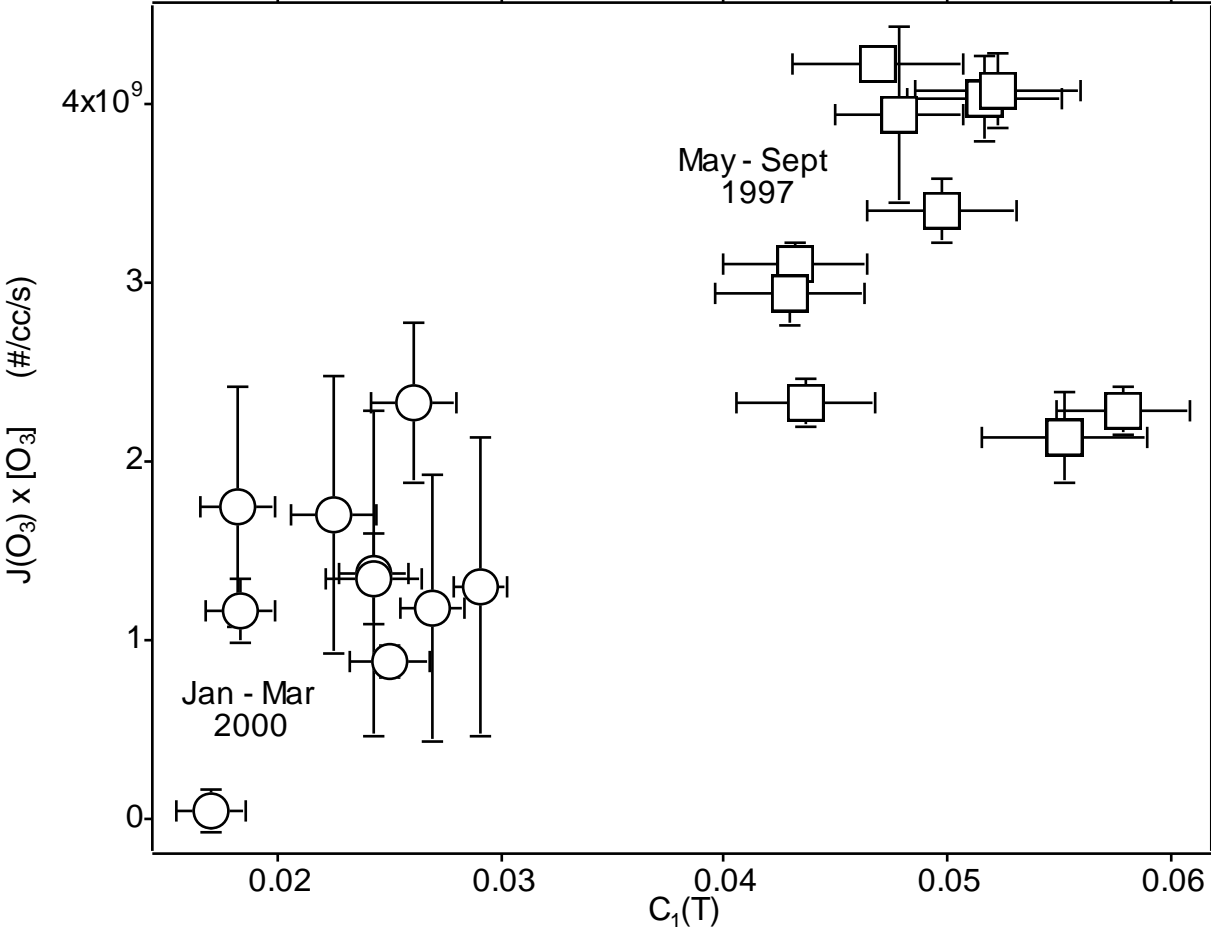
Correlation of H for ER-2 wind speed and temperature with jet strength



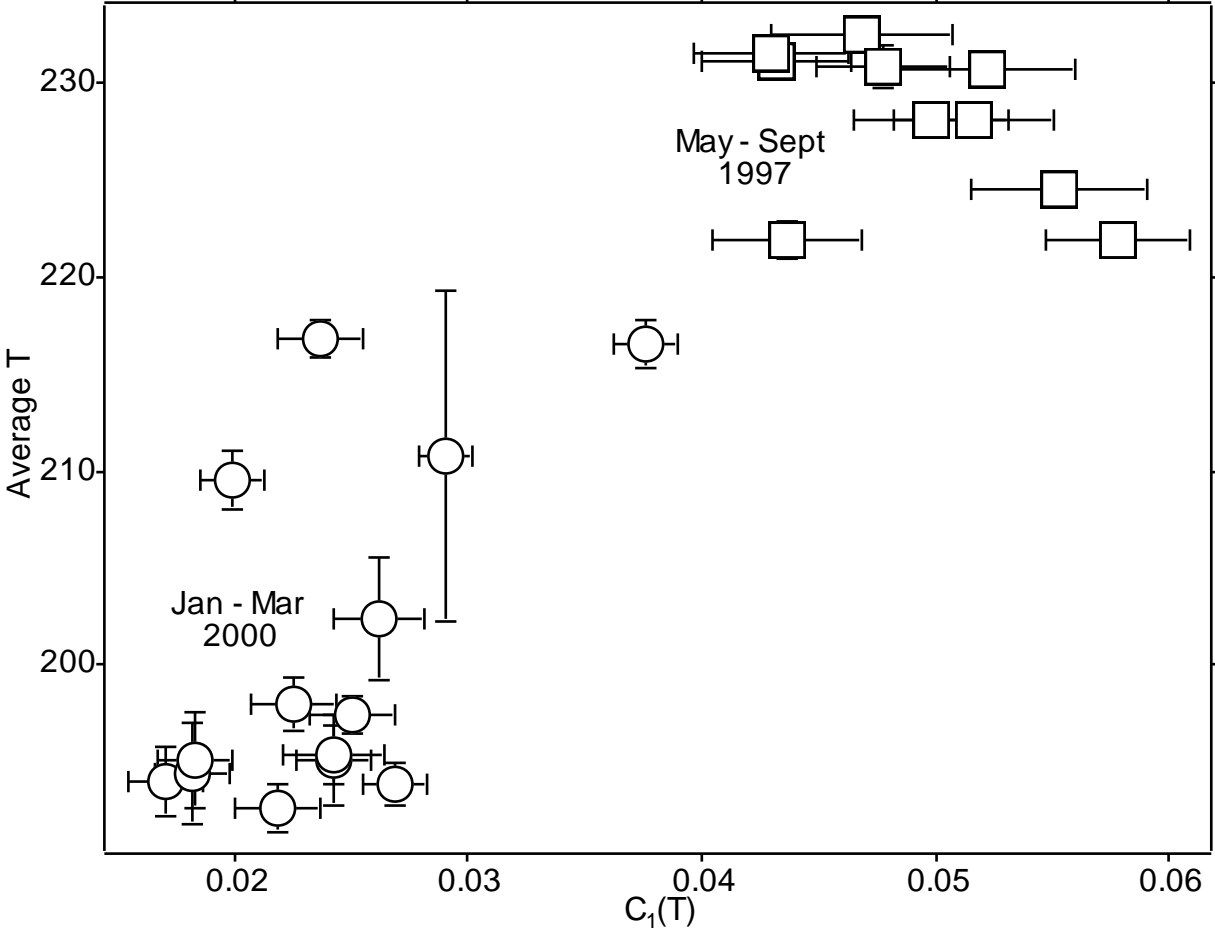
Correlation of H for dropsonde wind speed with jet strength, WS 2004



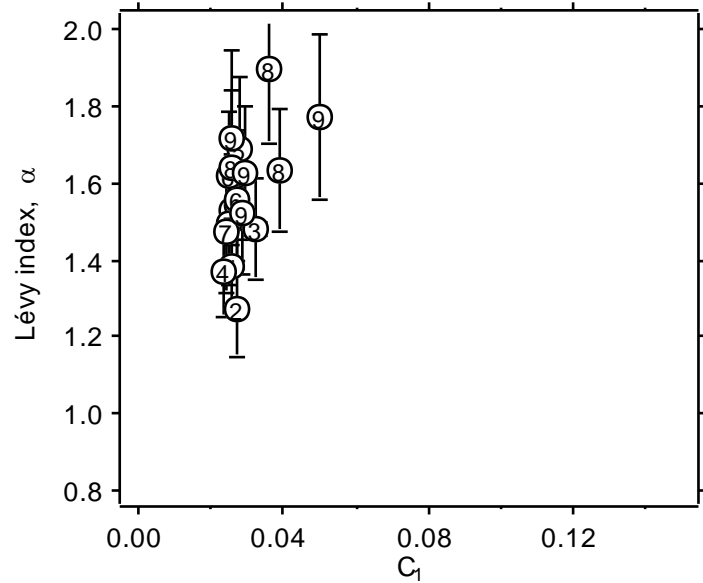
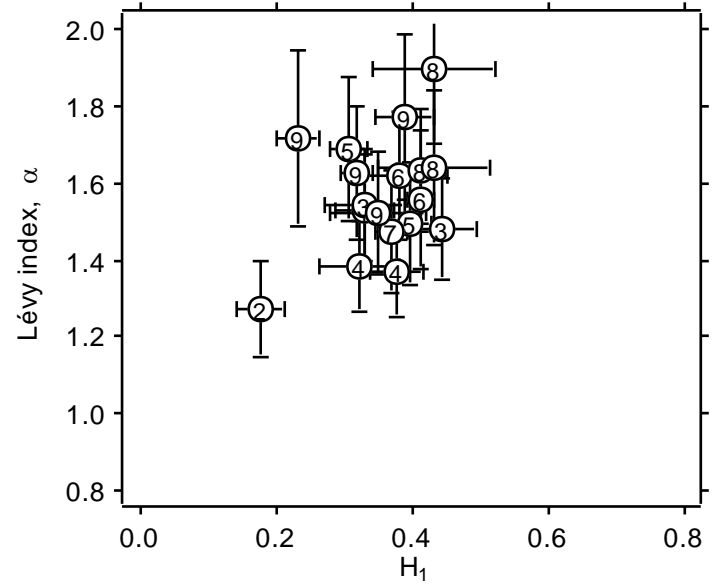
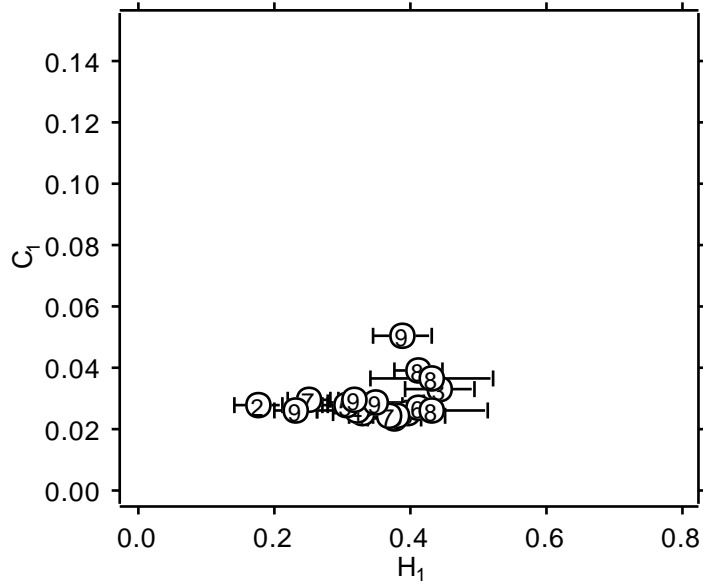
Correlation of the observed photodissociation rate of ozone with the intermittency of observed temperature. Arctic summer 1997 and winter 2000.



Correlation of average temperature along an ER-2 flight segment with its intermittency. Arctic summer 1997 and winter 2000.



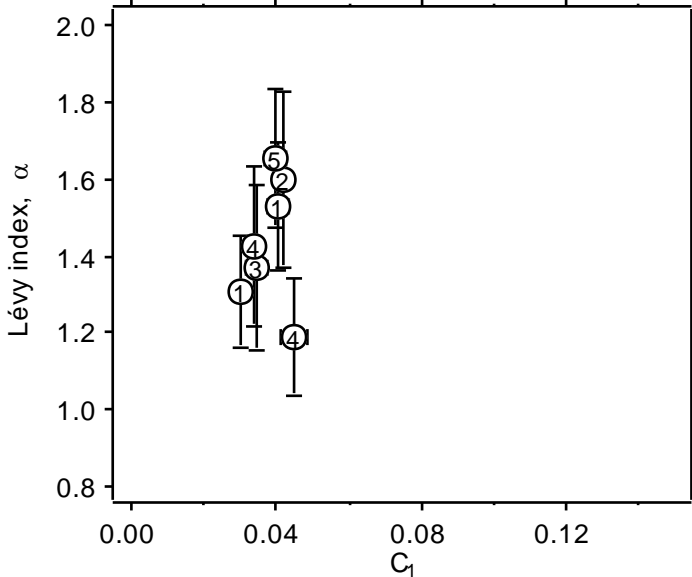
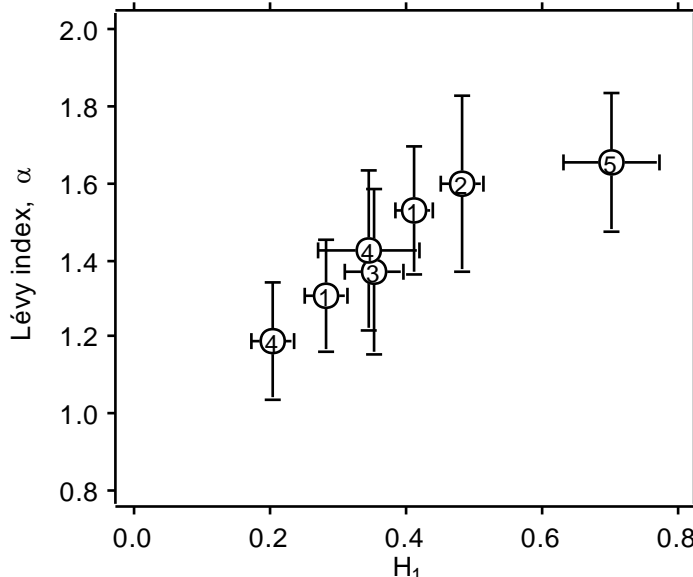
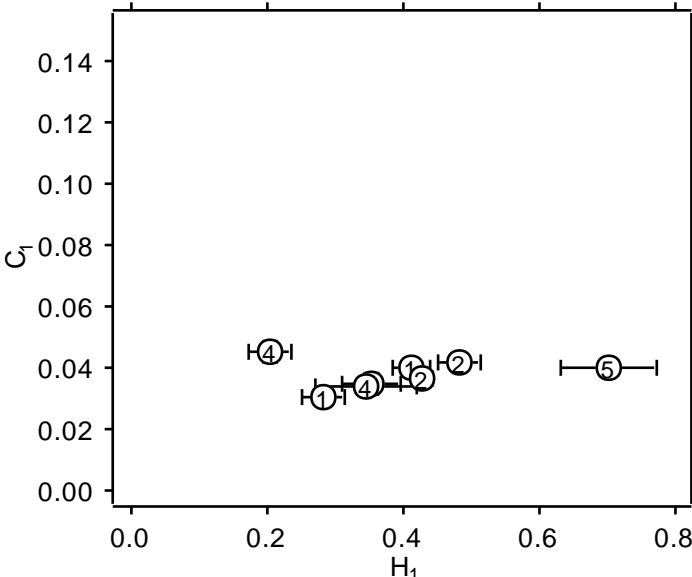
ER-2, O₃ SOLVE data. Scaling exponents H_1 , C_1 and α .



Dates

1	20000120
2	20000123
3	20000131
4	20000202
5	20000226
6	20000305
7	20000307
8	20000311
9	20000312

ER-2, O₃ scaling exponents, AAOE, Antarctic vortex, Aug-Sep 1987.



- Dates
- 1 19870830
 - 2 19870902
 - 3 19870904
 - 4 19870909
 - 5 19870922

Correlations among scaling exponents

- * H (wind speed) correlated with measures of jet stream strength, horizontally and vertically.
- * Intermittency of T correlated with O_3 photodissociation rate and T itself.
- * $H(O_3)$ correlated with $\alpha(O_3)$ in Antarctic and Arctic vortices - ozone conservation exponent correlated with multifractality exponent.

What to do about it?

- * Further work to make scale invariance theory more complete.
- * Better observations of $J[O_3]$ and T .
- * Molecular dynamics simulations of vortex photochemistry.
- * Can models pass the tests?

Overpopulation of high-speed molecules relative to Maxwell-Boltzmann

- * Effect on spectroscopic line shapes in wings and hence radiative transfer.
- * Effect on chemical kinetics.

What to do about it?

- * Experiments, e.g. vary $[O_3]$ and $[H_2O]$ with and without ozone photodissociation while taking high resolution spectra.
- * Molecular beam experiments with velocity PDF measurement in air - difficult!
- * See if translationally hot $O(^3P)$ atoms accelerate atmospheric chemistry. Do they scramble isotope fractionation?
- * Effect should accelerate reactions with an activation energy, and decelerate those with a negative temperature dependence, e.g. radical - radical recombinations.

Formal equivalences between **scale invariant** (r.h.s.)
and **statistical thermodynamic** (l.h.s.) variables

$$T = 1/qk_{\text{Boltzmann}}$$

temperature

$$f = e^{-K(q)}$$

partition function

$$G = -K(q)/q$$

Gibbs free energy

This offers possible links:

molecular scale



statistical thermodynamics



macroscopic scale invariant observables

Lecture 5.2: Key points and what next?

Summary

THE GAS CONSTANT R IS INSUFFICIENT FOR ATMOSPHERIC RESEARCH