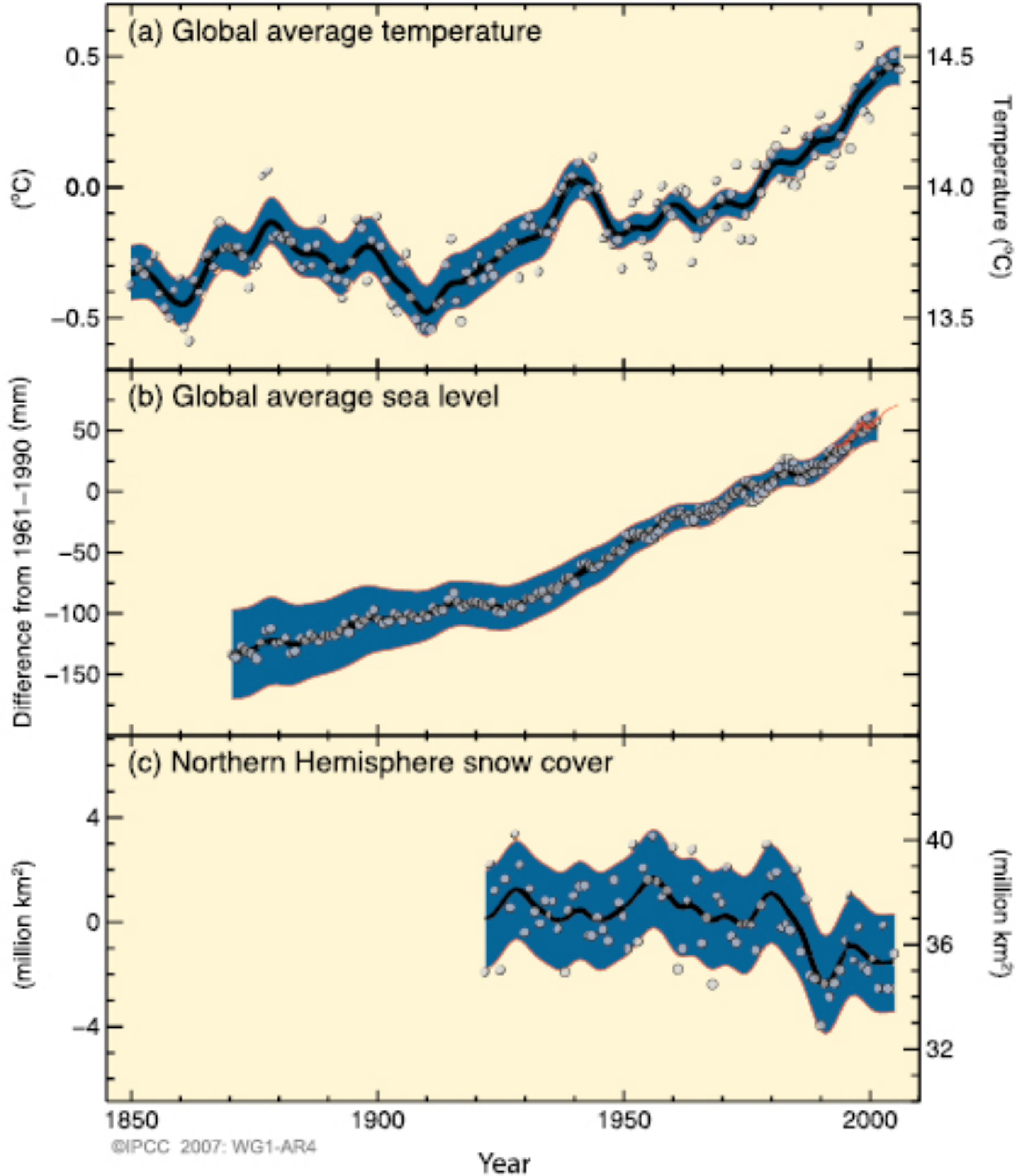
Reactive particles in the Pencil-Code

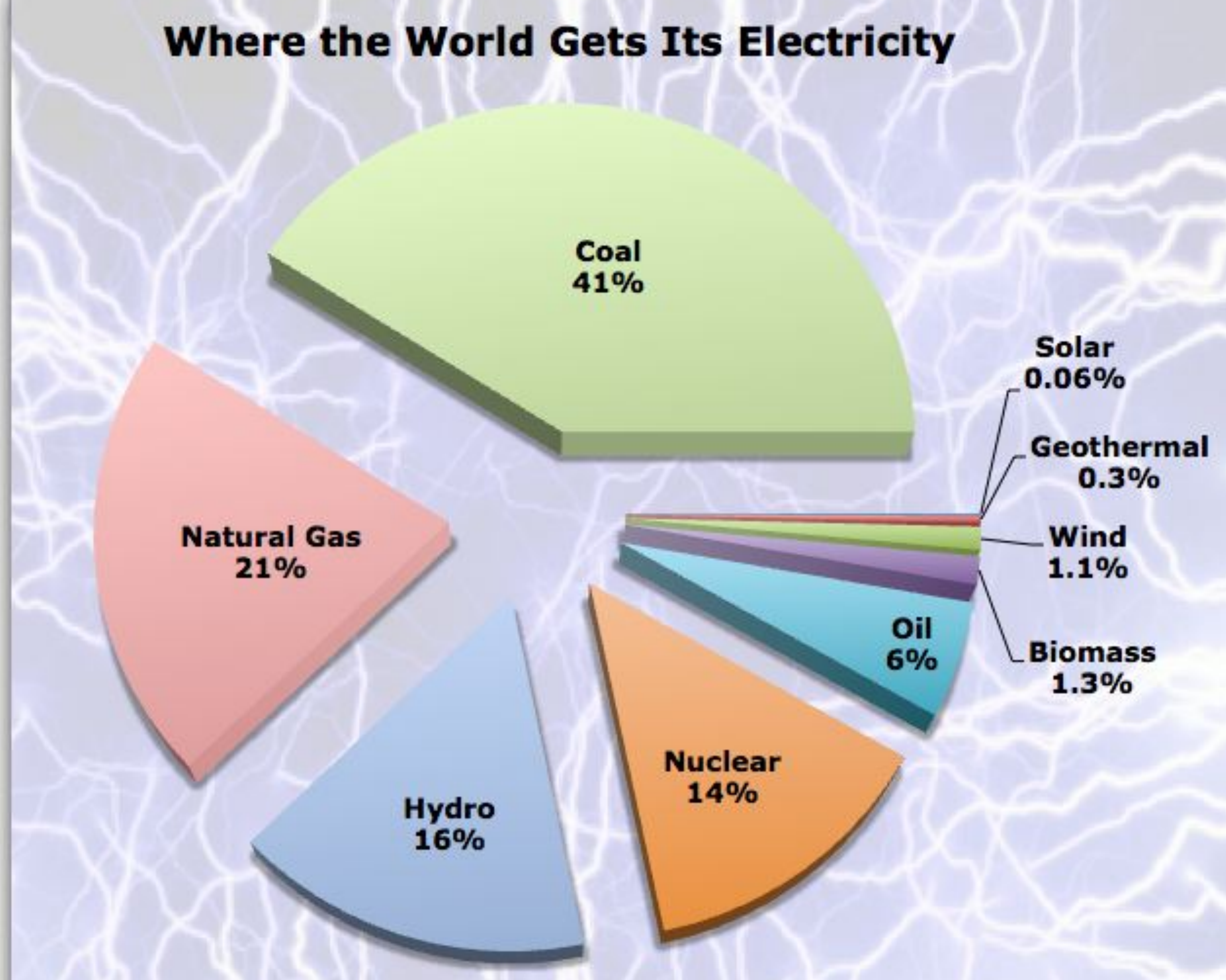
Gøttingen,

2014.07.08

Elect

- Esse
  - ligh
  - ref
  - qu
- 25% … to electr
- 38% … nass for >80%
- Energ




Where the World Gets Its Electricity
Coal
41%
Natural Gas
21%
Hydro
16%
Nuclear
14%
Oil
6%
Solar
0.06%
Geothermal
0.3%
Wind
1.1%
Biomass
1.3%

Turbulence – reactive particle coupling

- The effect of turbulence on heterogeneously reacting particles **is not known**
  - Relative particle velocity will yield changes in heat and mass transfer for particle with Stefan flow
  - "Fresh" fluid will flush the particles to increase reaction rate
  - Particle clustering will cause high local concentrations of products, which yields lower reaction rate

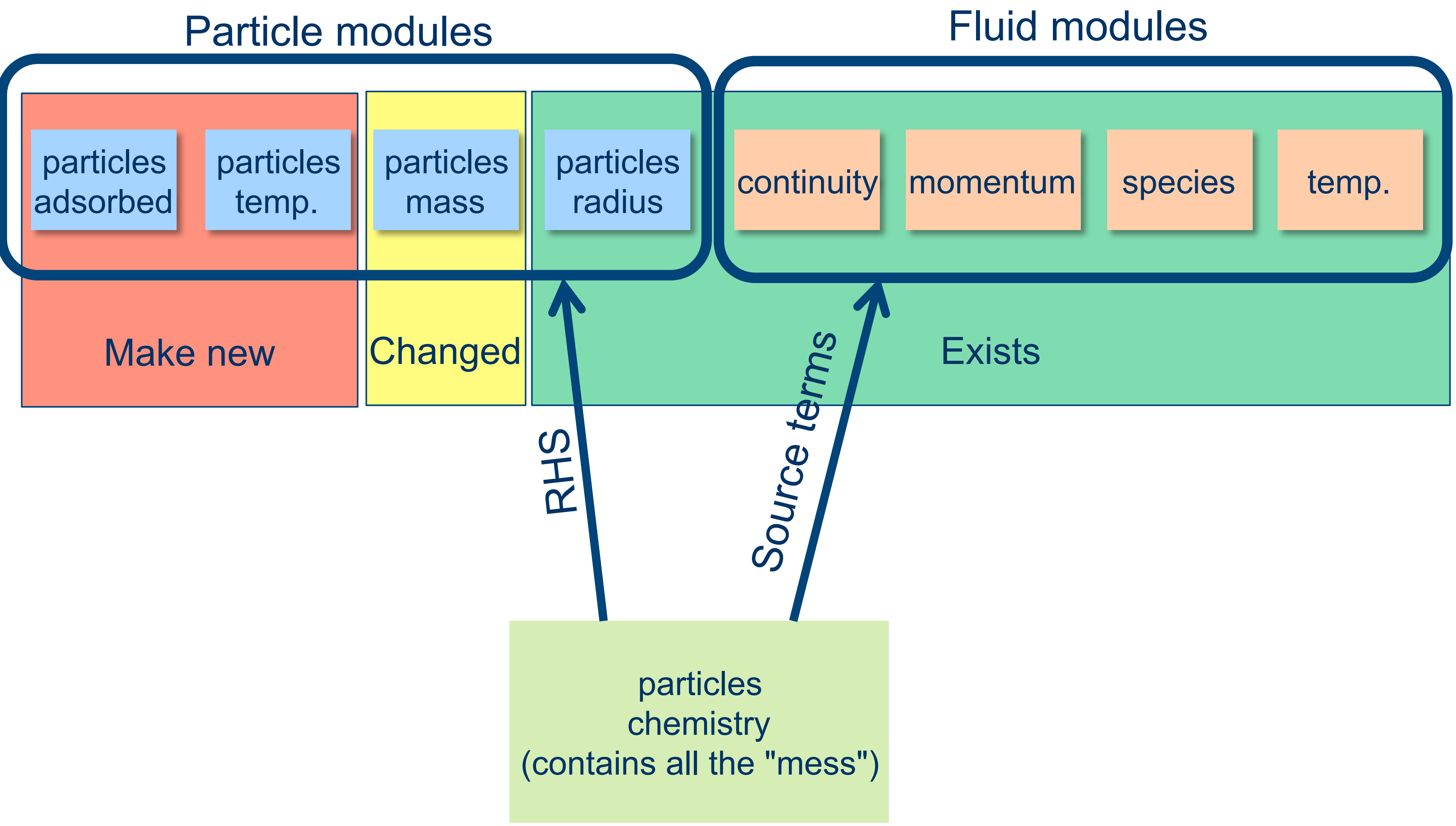
Two levels of study

- Level I: fully resolved particle
  - One, or a few, particles in flow with constant relative velocity
  - Find Nusselt and Sherwood number for moving particles with Stefan flow
  - Identify the optimal boundary layer treatment (single or double)
  - Use the immersed boundary method to model a reactive particle
  - Will implement model for particle temperature and species production
- Level II: large cloud of Lagrangian point particles
  - Require Nusselt and Sherwood numbers
  - Require boundary layer treatment
  - Will be used to study the effect of turbulence on cloud of particles

Implementation of reactive point particles

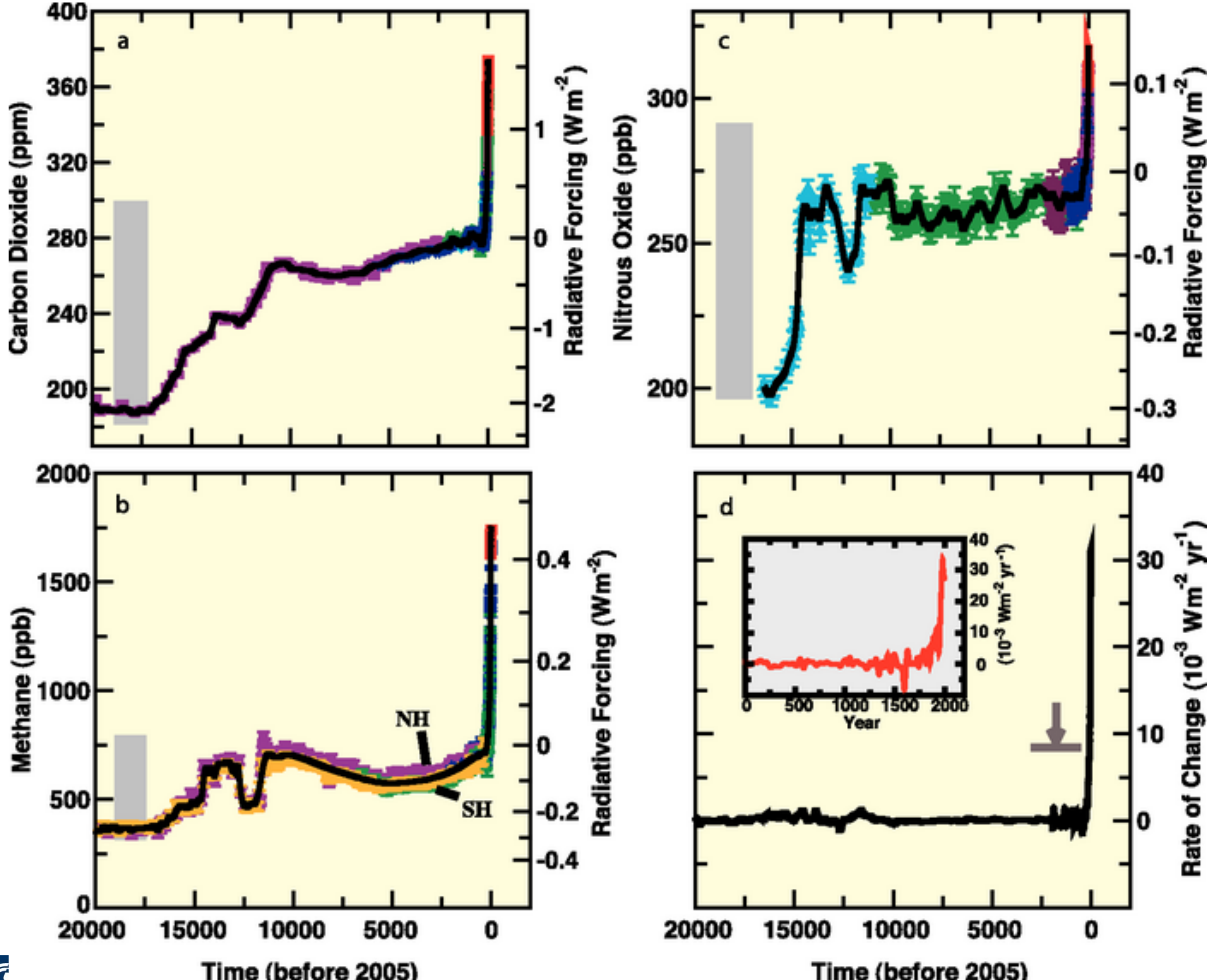
- Source terms in fluid equations:
  - continuity
  - momentum
  - temperature
  - species mass fractions
- Modifications to existing particle modules:
  - particles_radius
  - particles_mass
- New particle modules:
  - particles_temperature
  - particles_adsorbed_species
  - particles_chemistry (contains most of the "mess")

Code structure



Conclusion from the discussion

- Anders rename particles_mass to particles_density
- Let particles_chemistry (or the other particle modules if applicable) modify the df array of the fluid variables (such that the particle stuff is not visible in the fluid module)
- Othervise slide 7 is OK


a
Carbon Dioxide (ppm)
400
360
320
280
240
200
Radiative Forcing (Wm-2)
1
0
-1
-2
b
Methane (ppb)
2000
1500
1000
500
0
NH
SH
Radiative Forcing (Wm-2)
0.4
0.2
0
-0.2
-0.4
20000
15000
10000
5000
0
Time (before 2005)
c
Nitrous Oxide (ppb)
300
250
200
Radiative Forcing (Wm-2)
0.1
0
-0.1
-0.2
-0.3
d
40
30
20
10
0
(10-3 Wm-2 yr-1)
0
500
1000
1500
2000
Year
Rate of Change (10-3 Wm-2 yr-1)
40
30
20
10
0
20000
15000
10000
5000
0
Time (before 2005)