Understanding and predicting CO_2 properties

Richard Graham

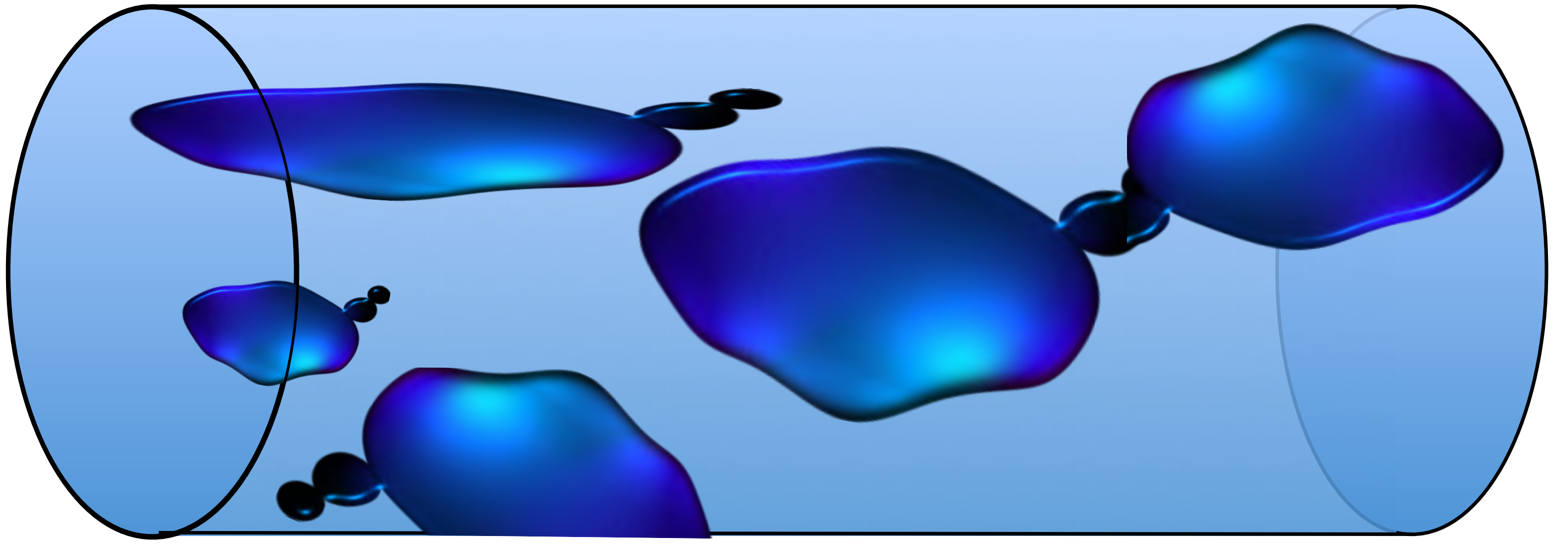
Tom Demetriades, Alex Cresswell, Martin Nelson,

Richard Wilkinson and Simon Preston

School of Mathematical Sciences, University of Nottingham.

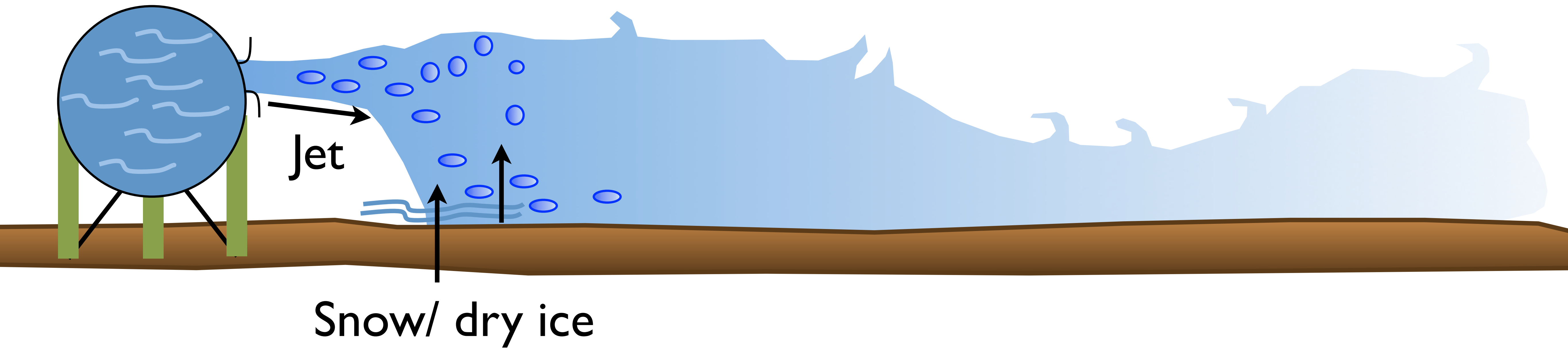
The University of Nottingham

Potential applications: Avoiding pipeline issues



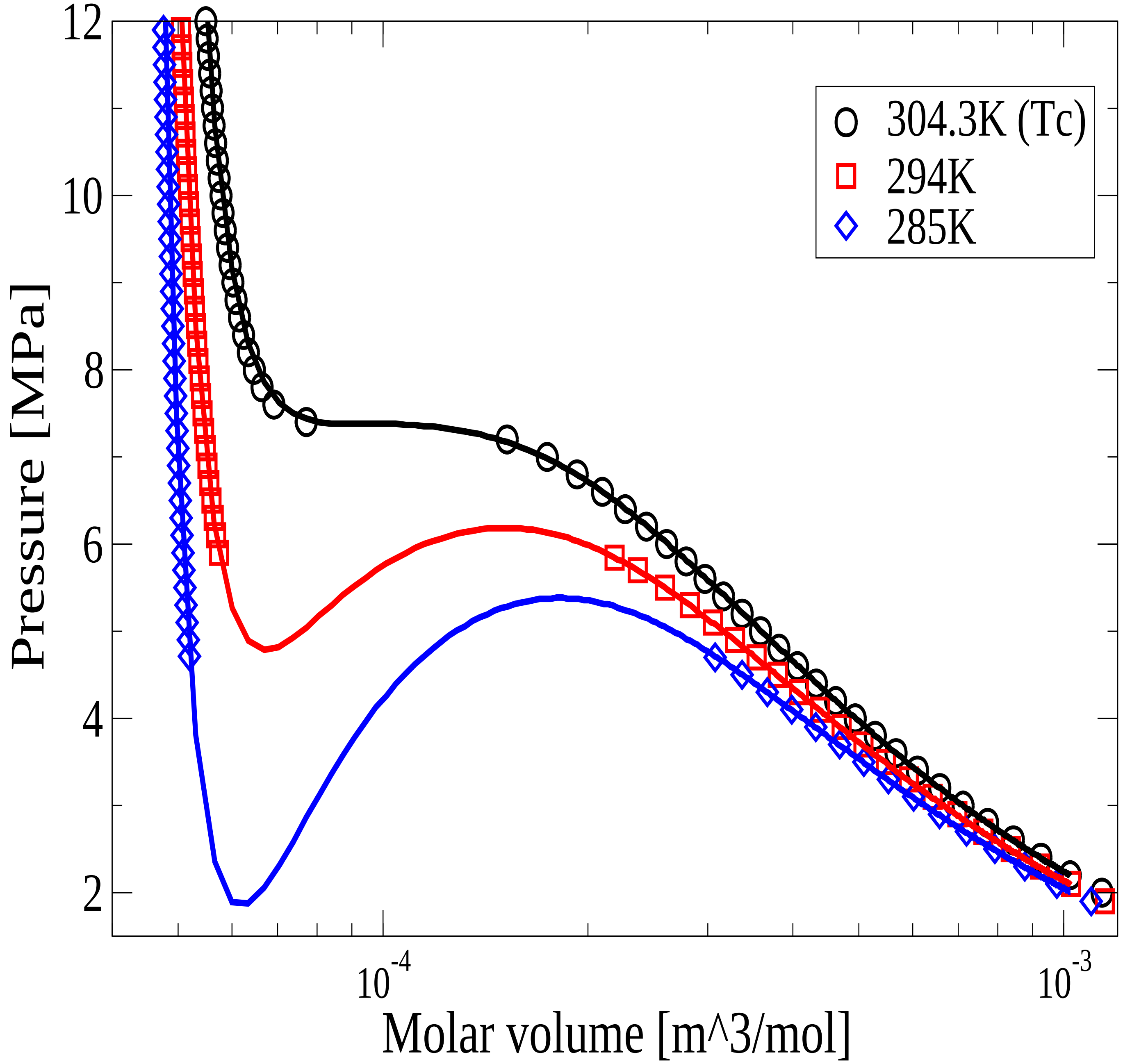
Two-phase flow

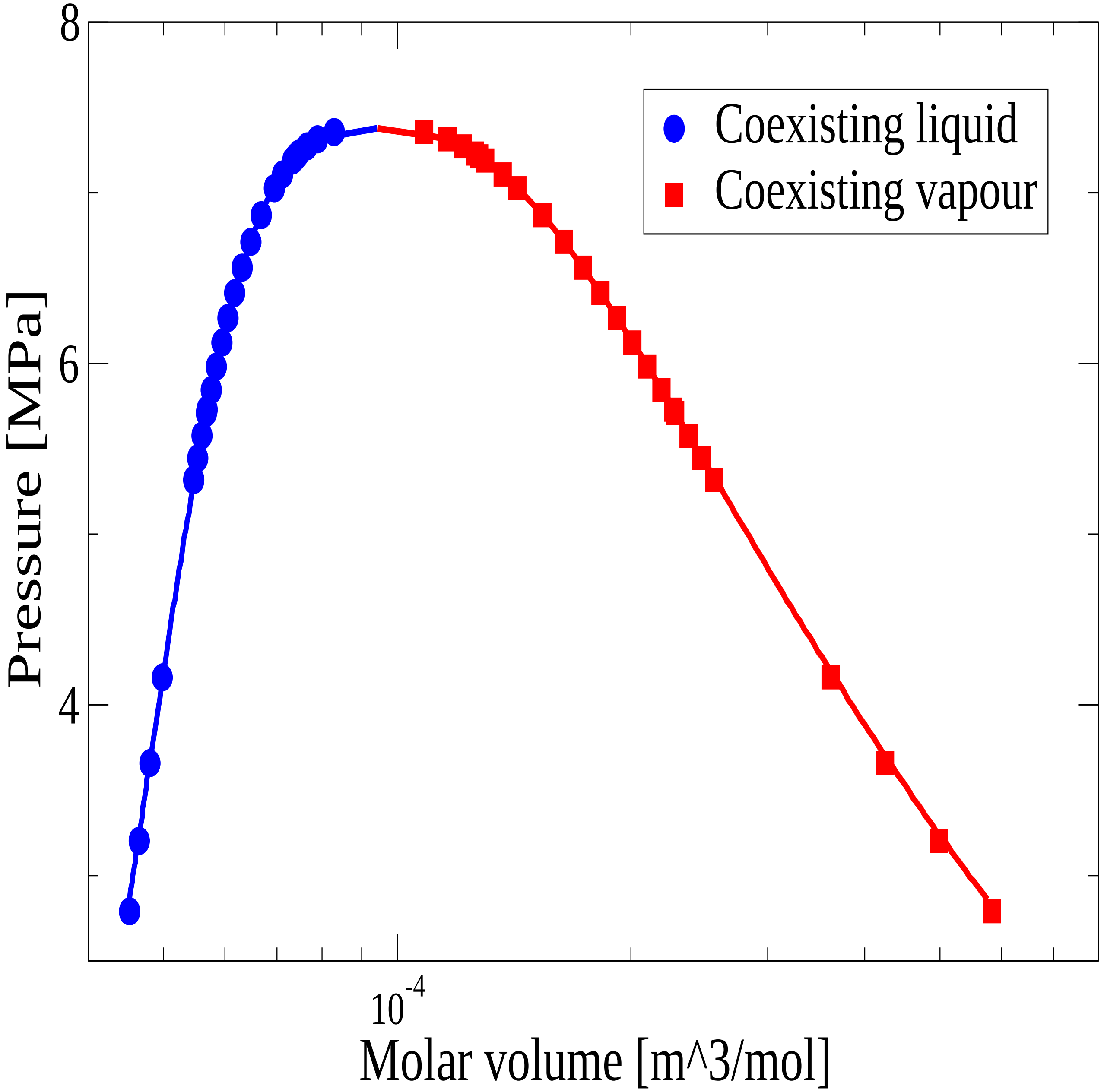
Pipe rupture



Predictions (pure CO2)

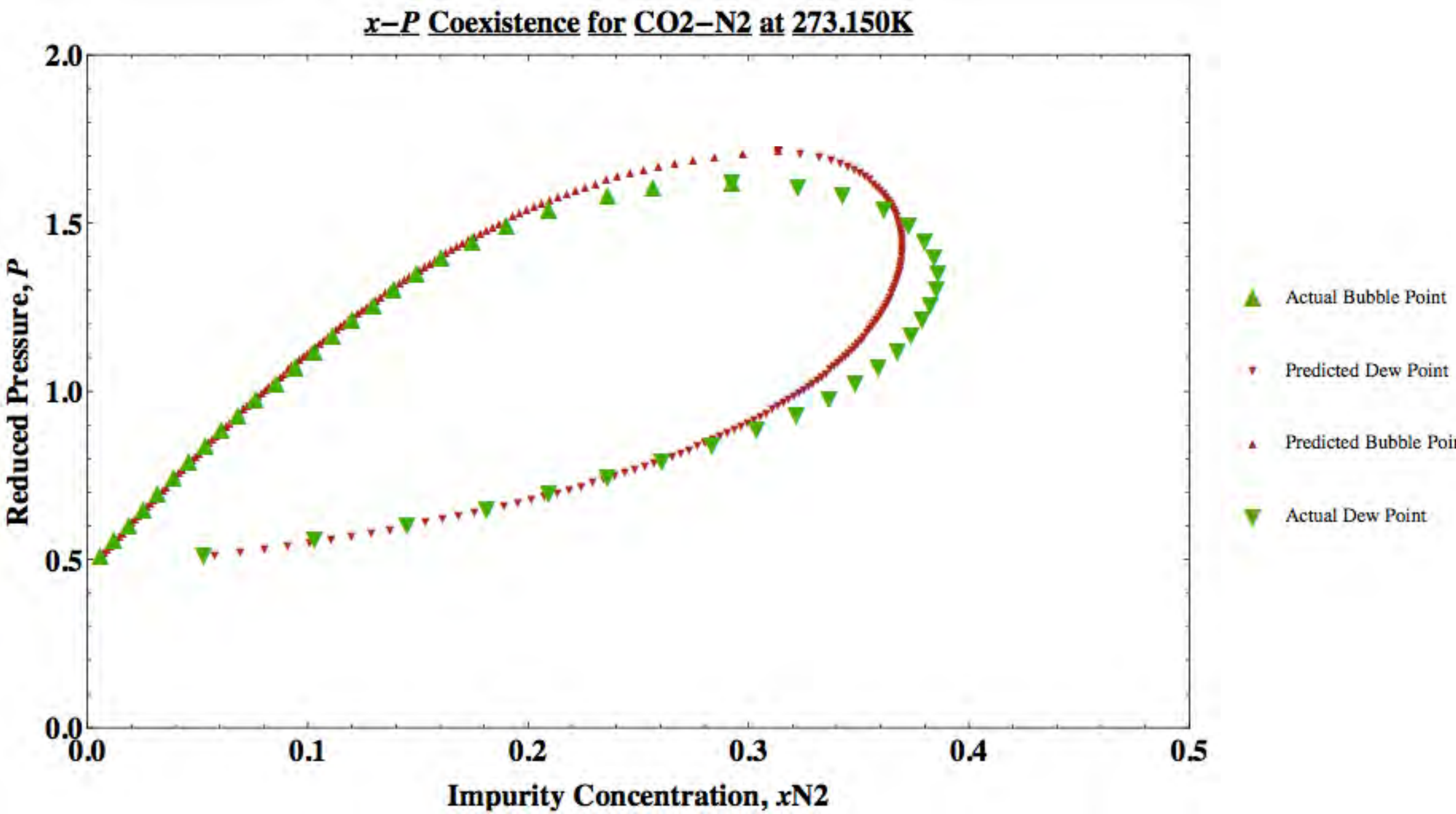
$$P(v,T) := \frac{RT}{v+a} - \frac{b}{v^2+c} - \frac{d}{v^3+e} + \left(\frac{f}{v-g}\right)^6$$



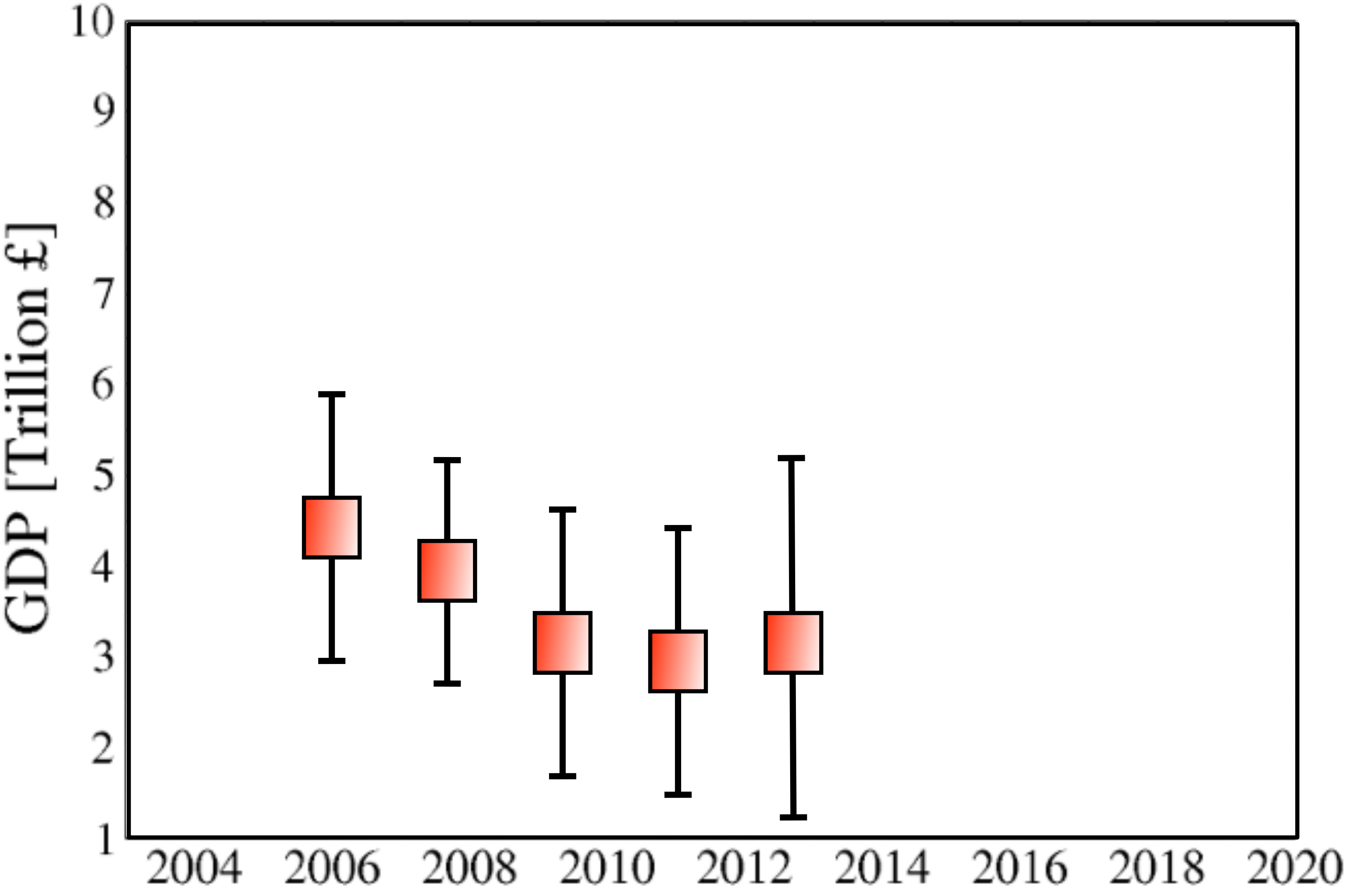


Mixture modelling

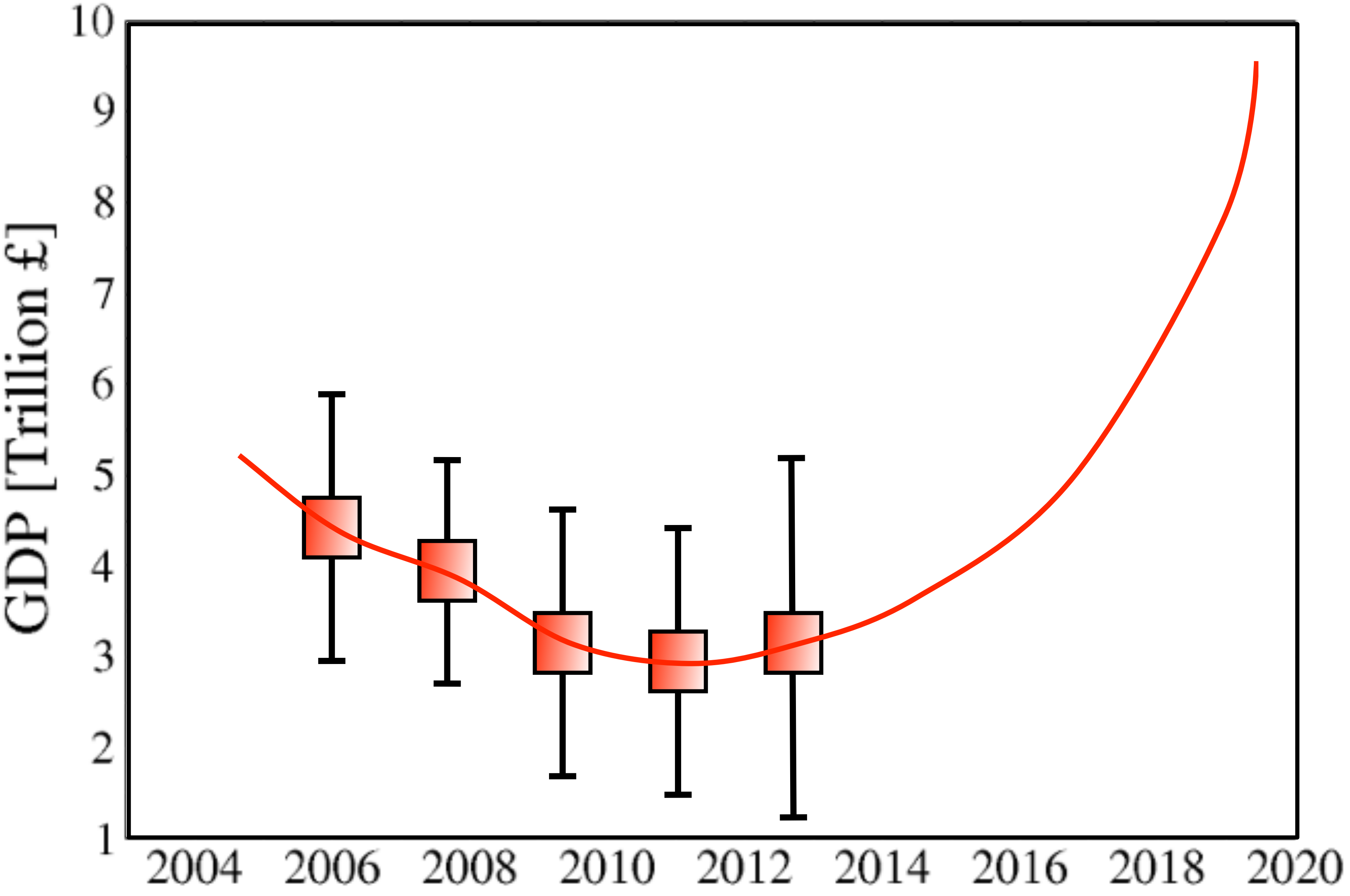
CO2+N2



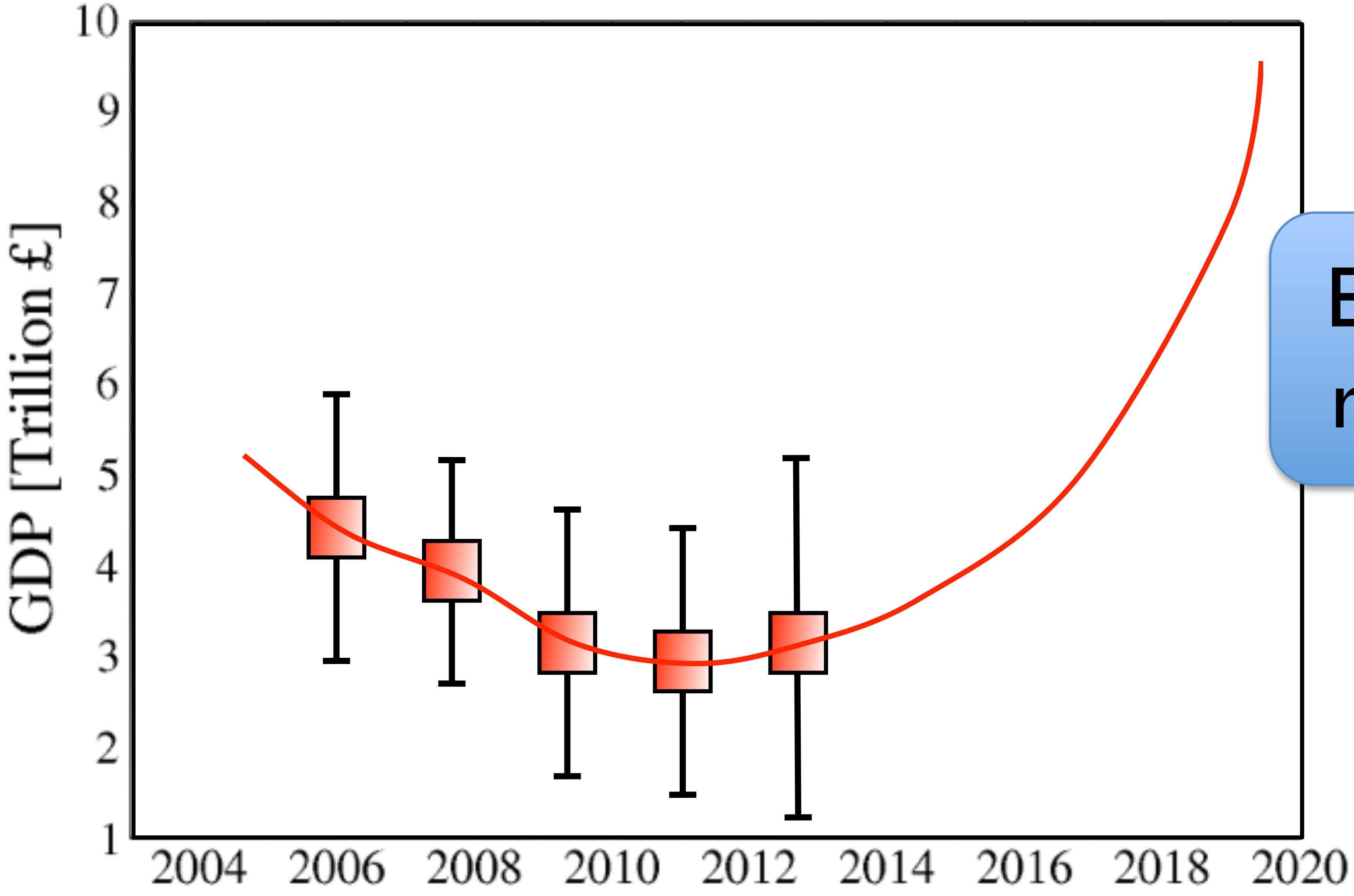
Uncertainty quantification

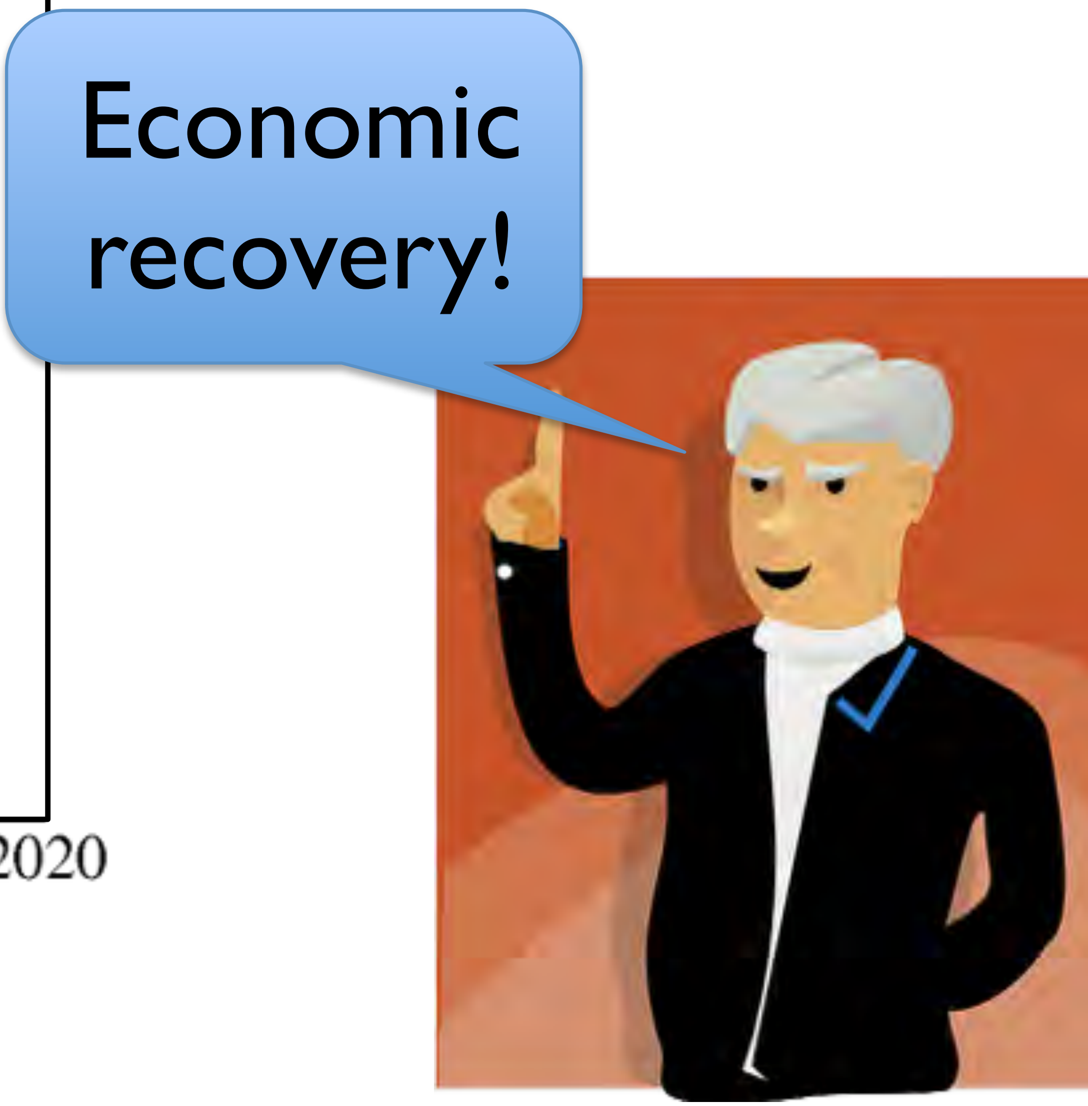


Uncertainty quantification

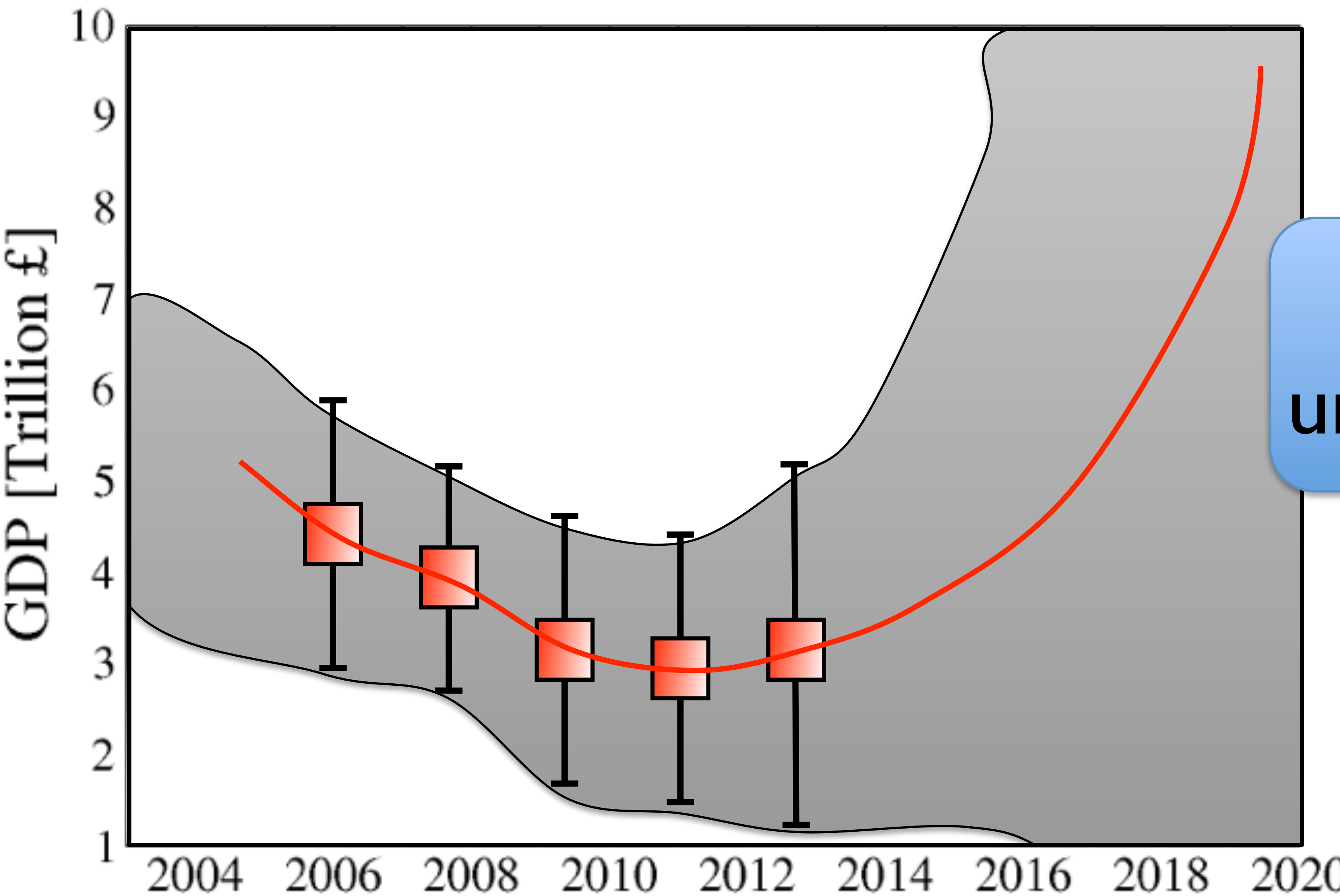


Uncertainty quantification



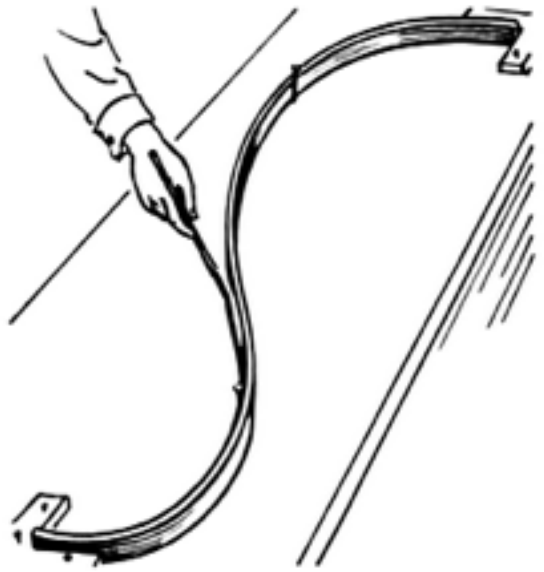


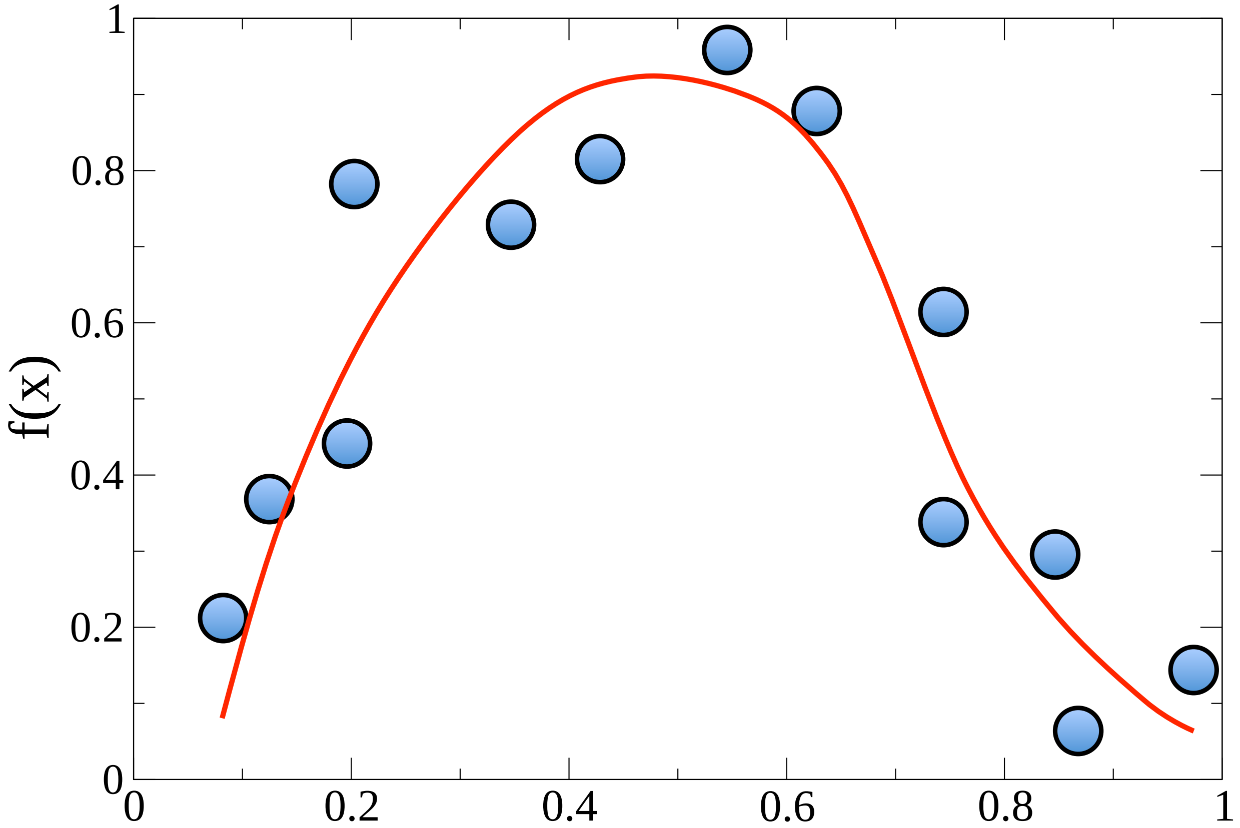
Uncertainty quantification



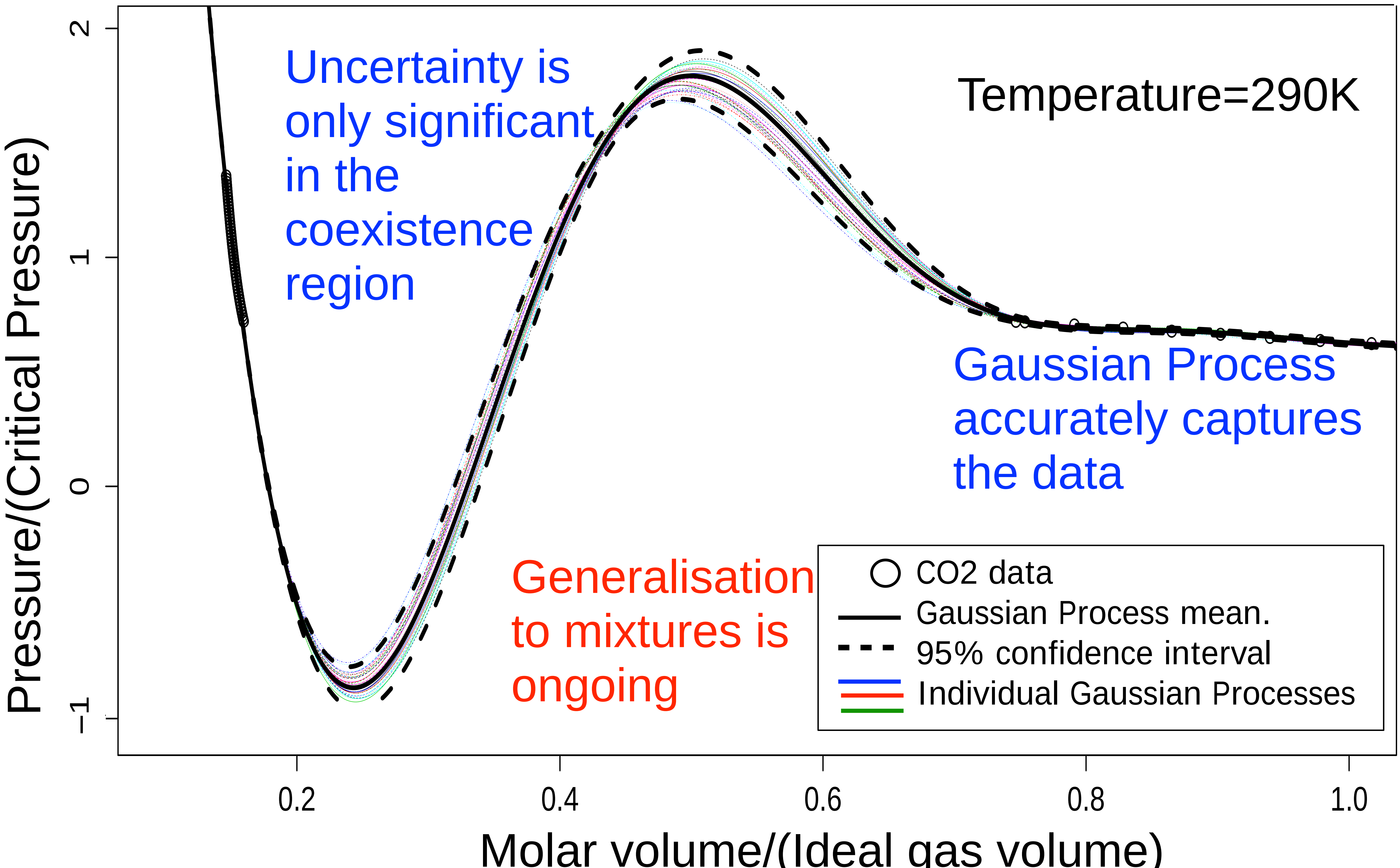
Introduction to non-parametric methods

- Model for **pressure against volume,** as with an equation of state.
- However, no need to specify **terms** or **parameters**
- Model '**learns**' the P(v) functional form **from the measurements**

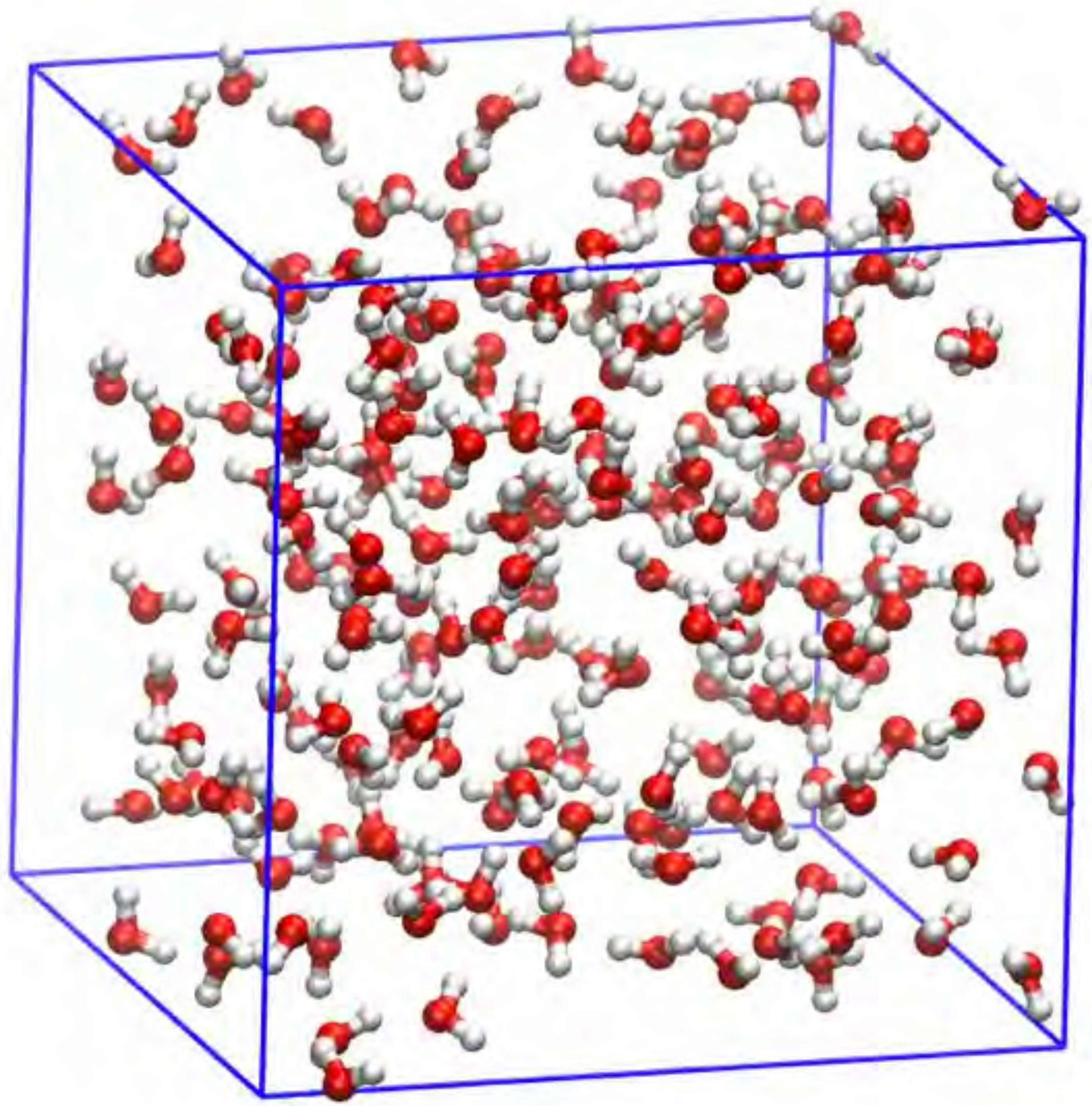




A Gaussian process for pure CO2



Molecular simulation



Computer model of individual molecules within a small box of fluid.

Can predict:

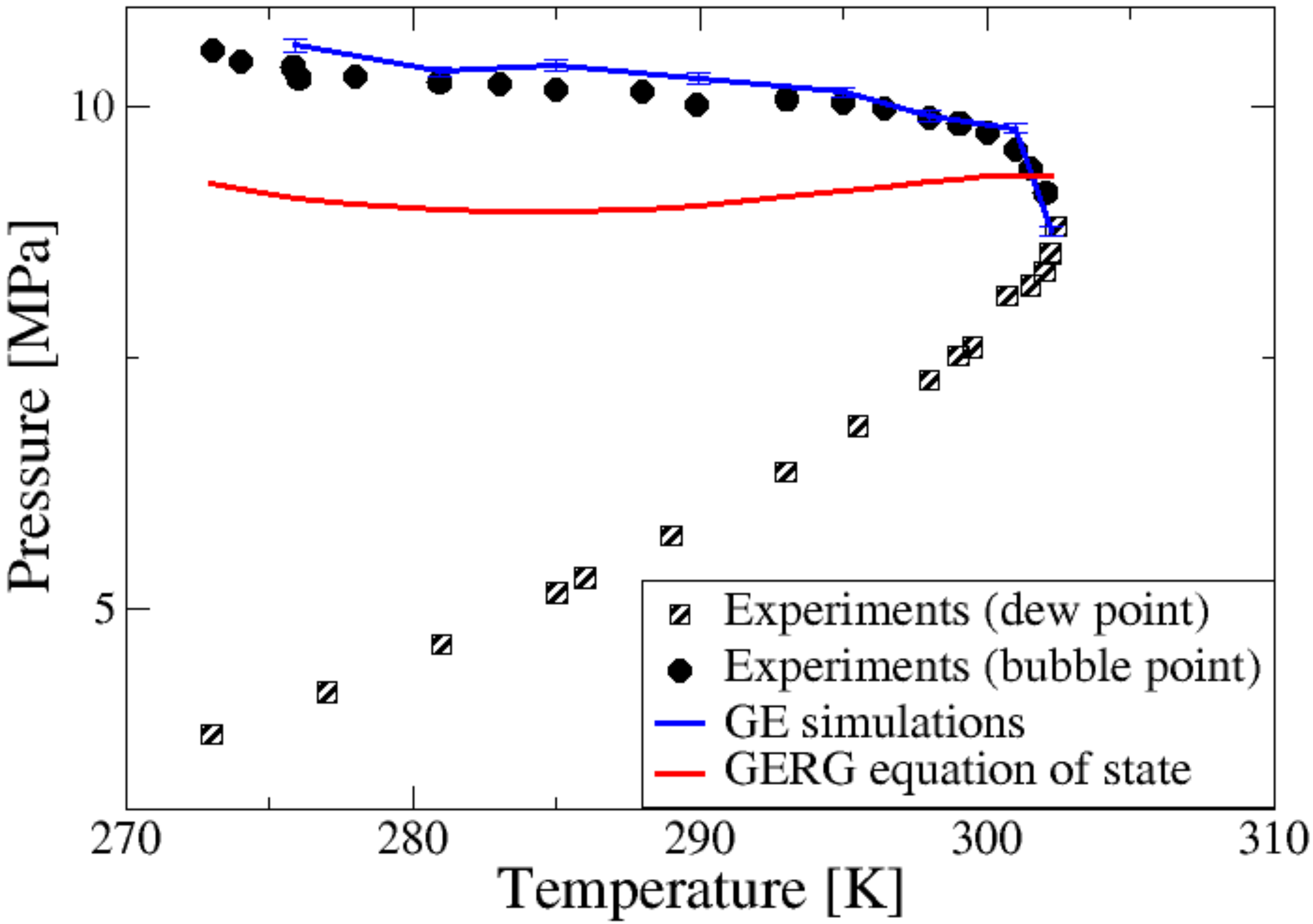
- Pressure-volume
- Coexistence
- Effect of impurity
- Most other quantities of interest

Can be used where experiments are unavailable?

Can be used to derive an Equation of State?

Bubble point comparison

CO_2 + 5%H_2



Phase boundary measurements by Jie Ke, Mike George et al