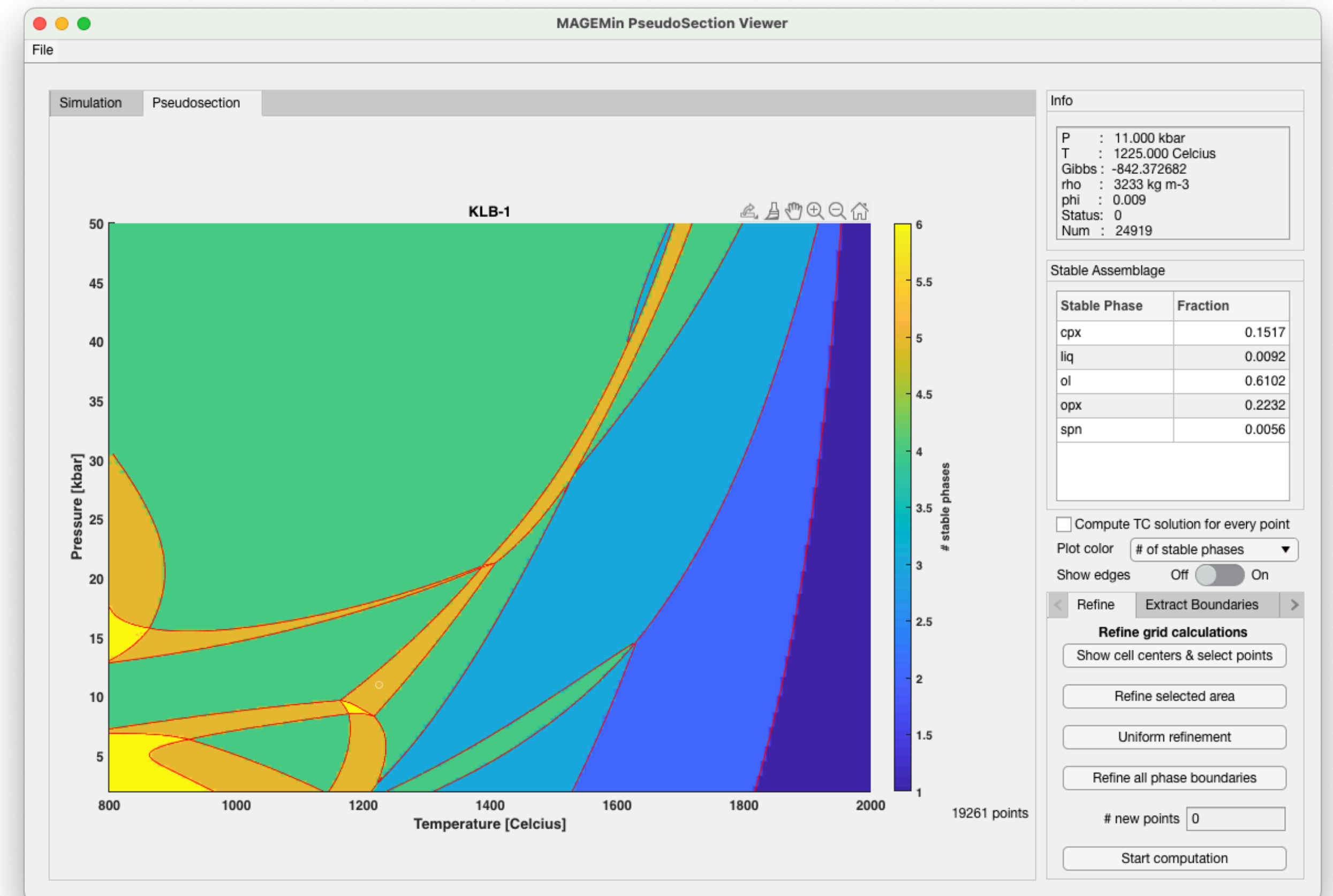


Neural networks, local minima and computational thermodynamics

Boris Kaus & Nicolas Riel
Johannes-Gutenberg University of Mainz

MAGEMin: example diagram

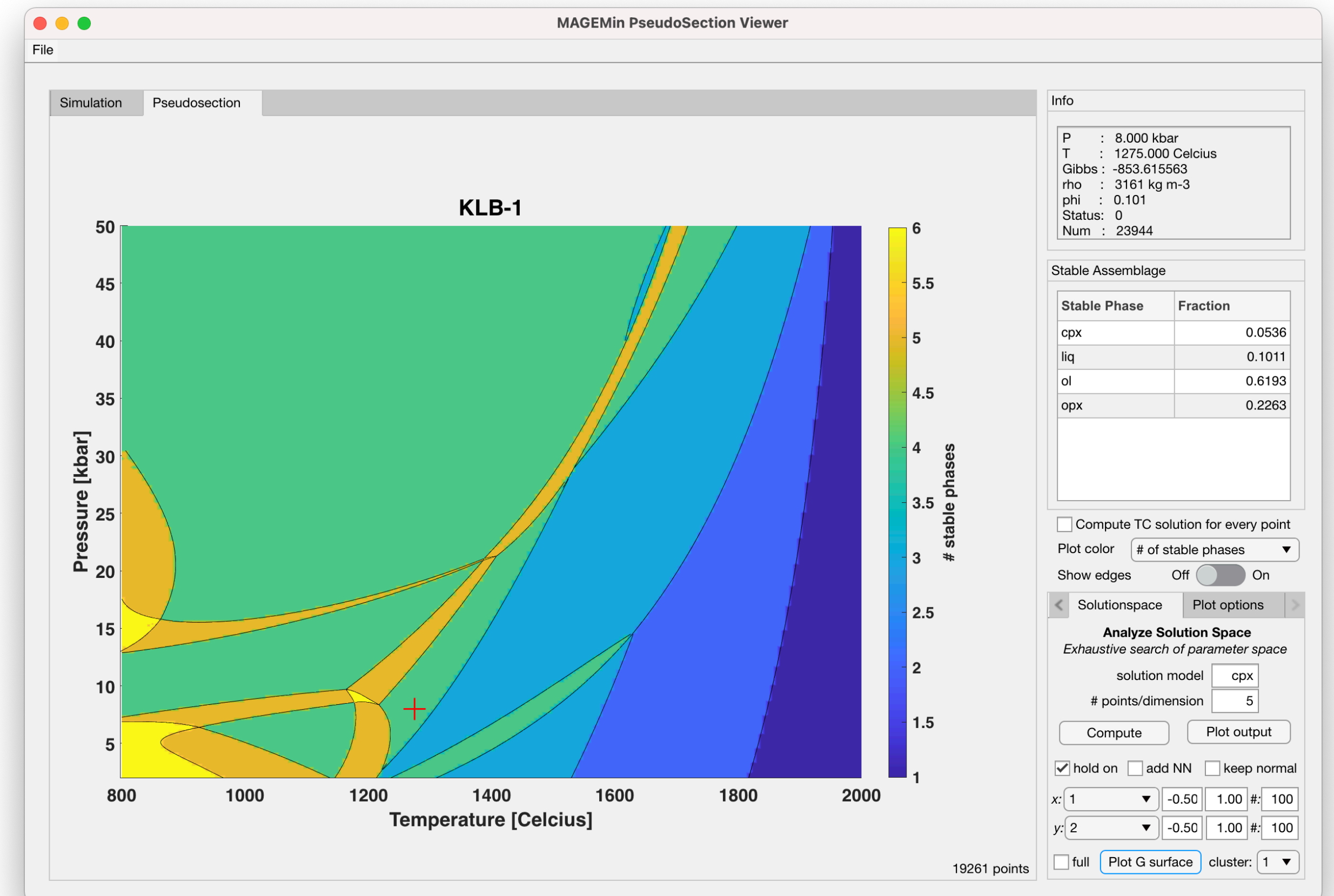
- KLB-1: Melting of dry peridotite
- Gibbs energy minimisation which gives the stable mineral assemblage as $f(T, P, \text{chemistry})$
- MAGEMin: new, parallel, approach (see presentation by *RIEL et al.*)
 - Red lines: THERMOCALC
 - Colored fields: MAGEMin
- Nonlinear optimization problem.



▸ **But how many local solutions exist?**

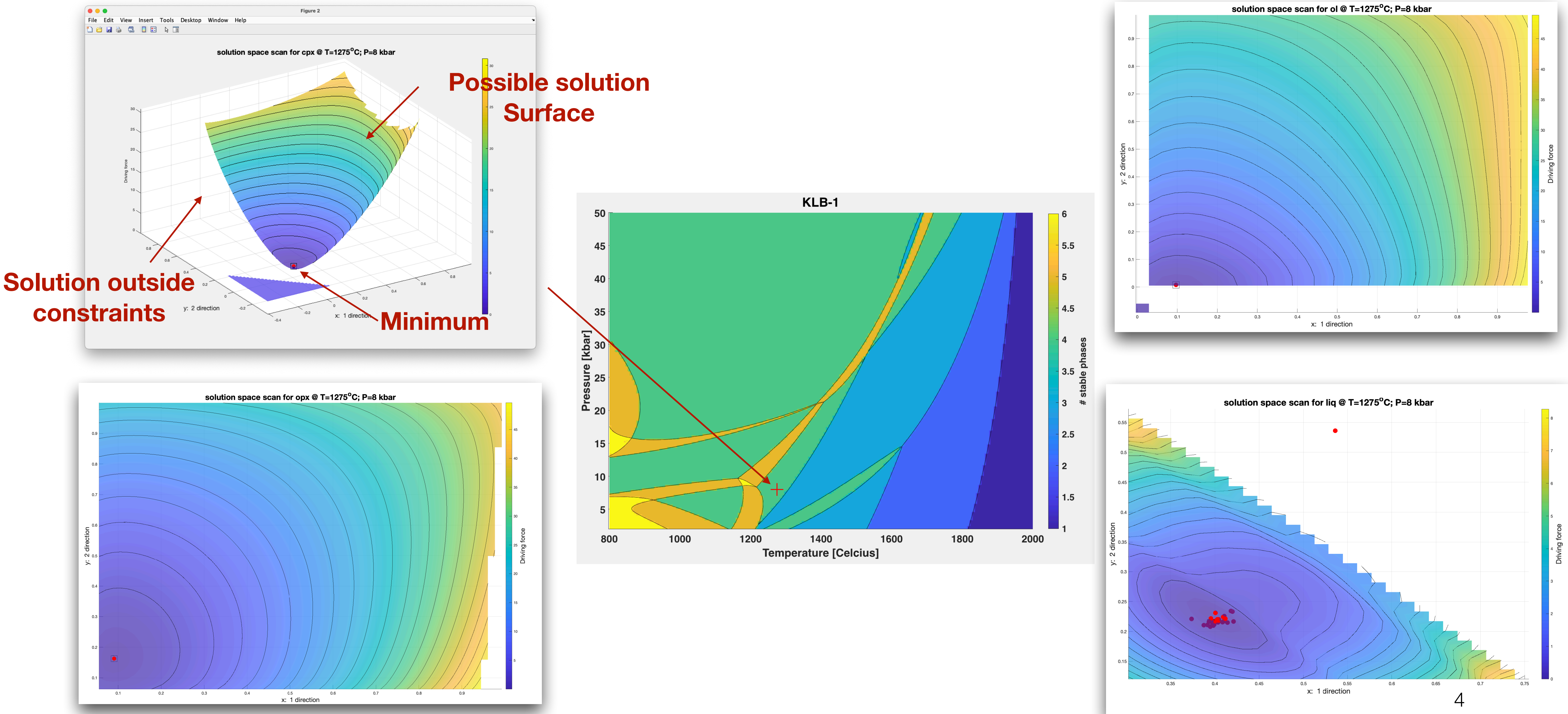
How many solutions are there?

- Let's check!
- Select a point & solution model
- Extract Γ @ equilibrium
- Sample the model space
- Compute driving force (=0 at equilibrium)



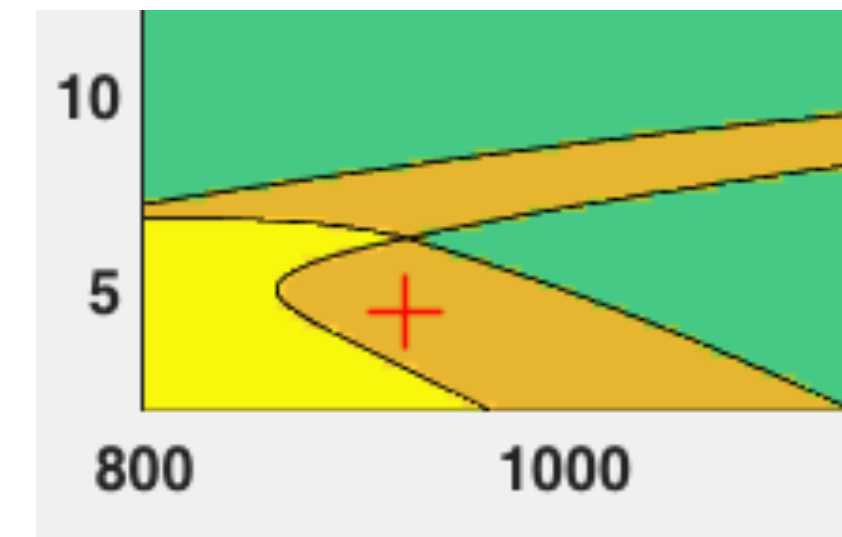
Coloured fields: MAgEMin results
Thin lines: ThermoCalc results

How many solutions are there?

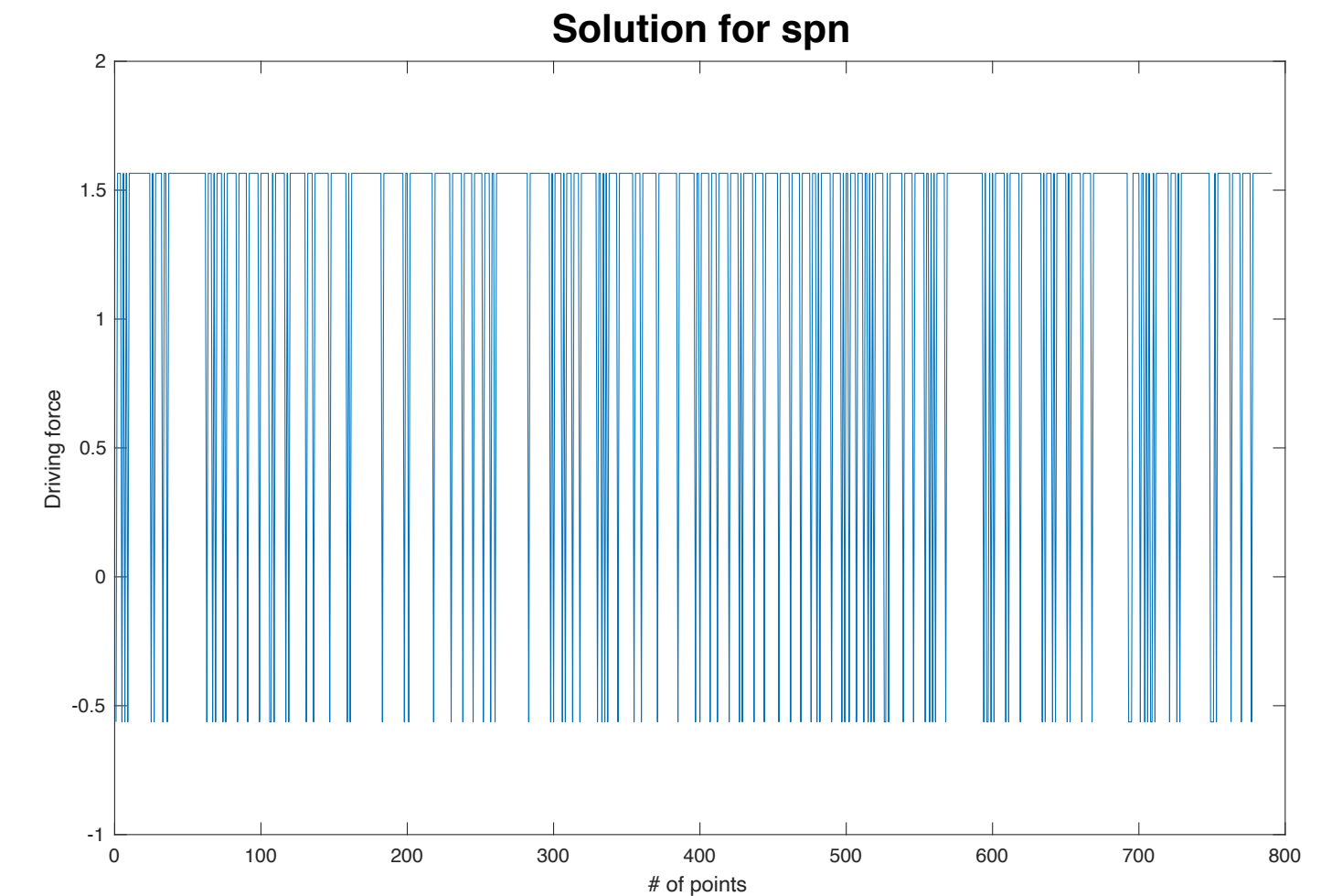
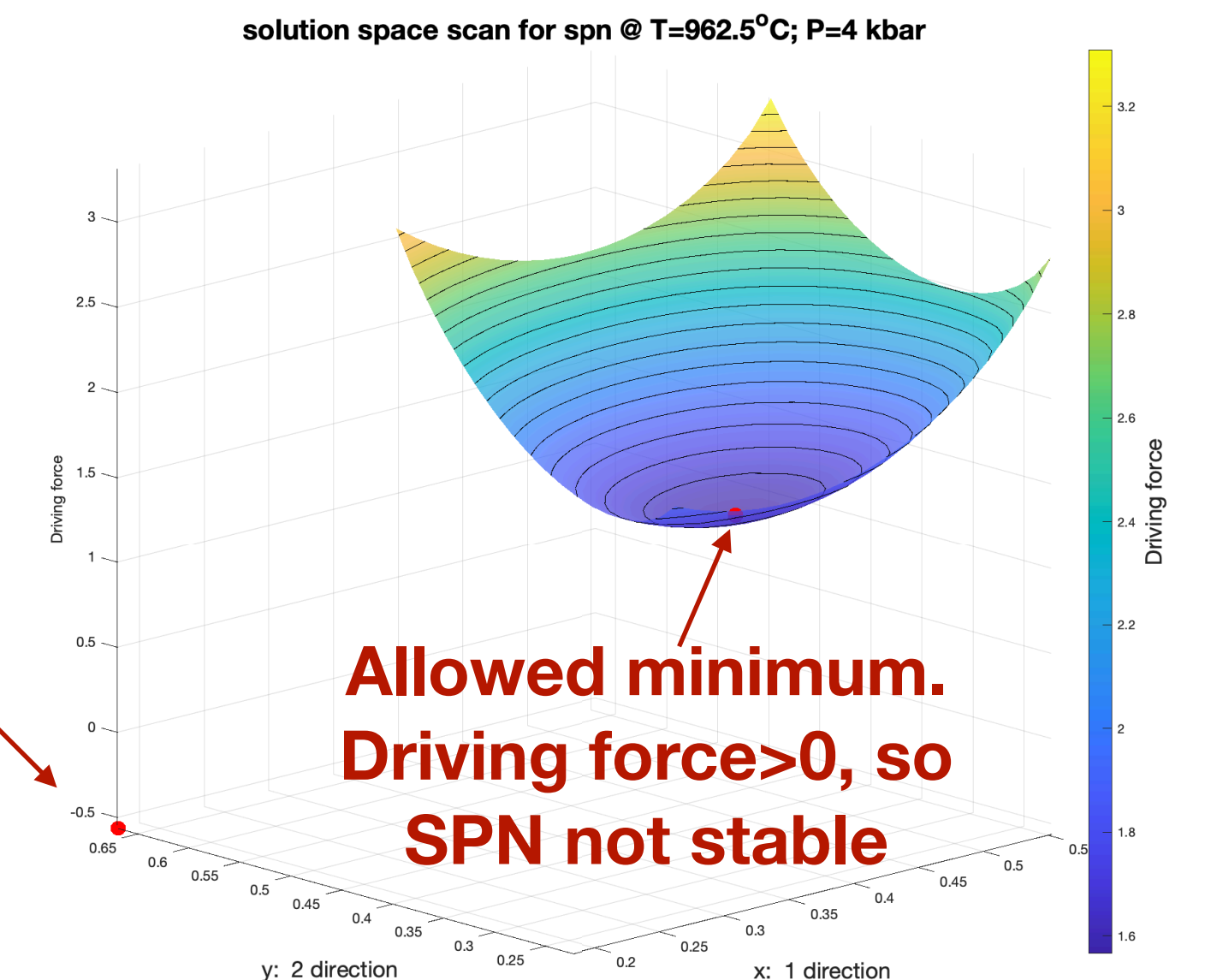


How many solutions are there?

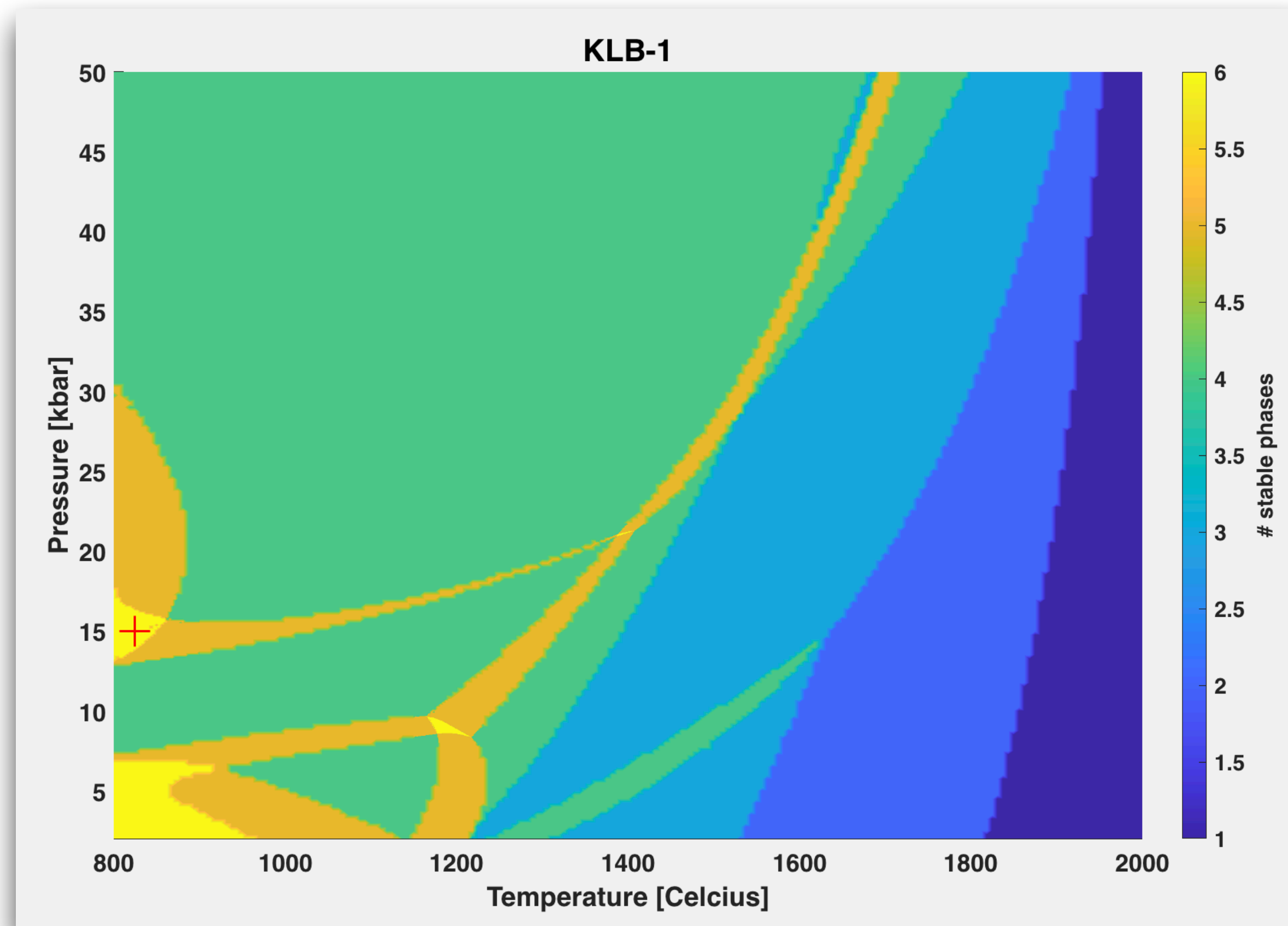
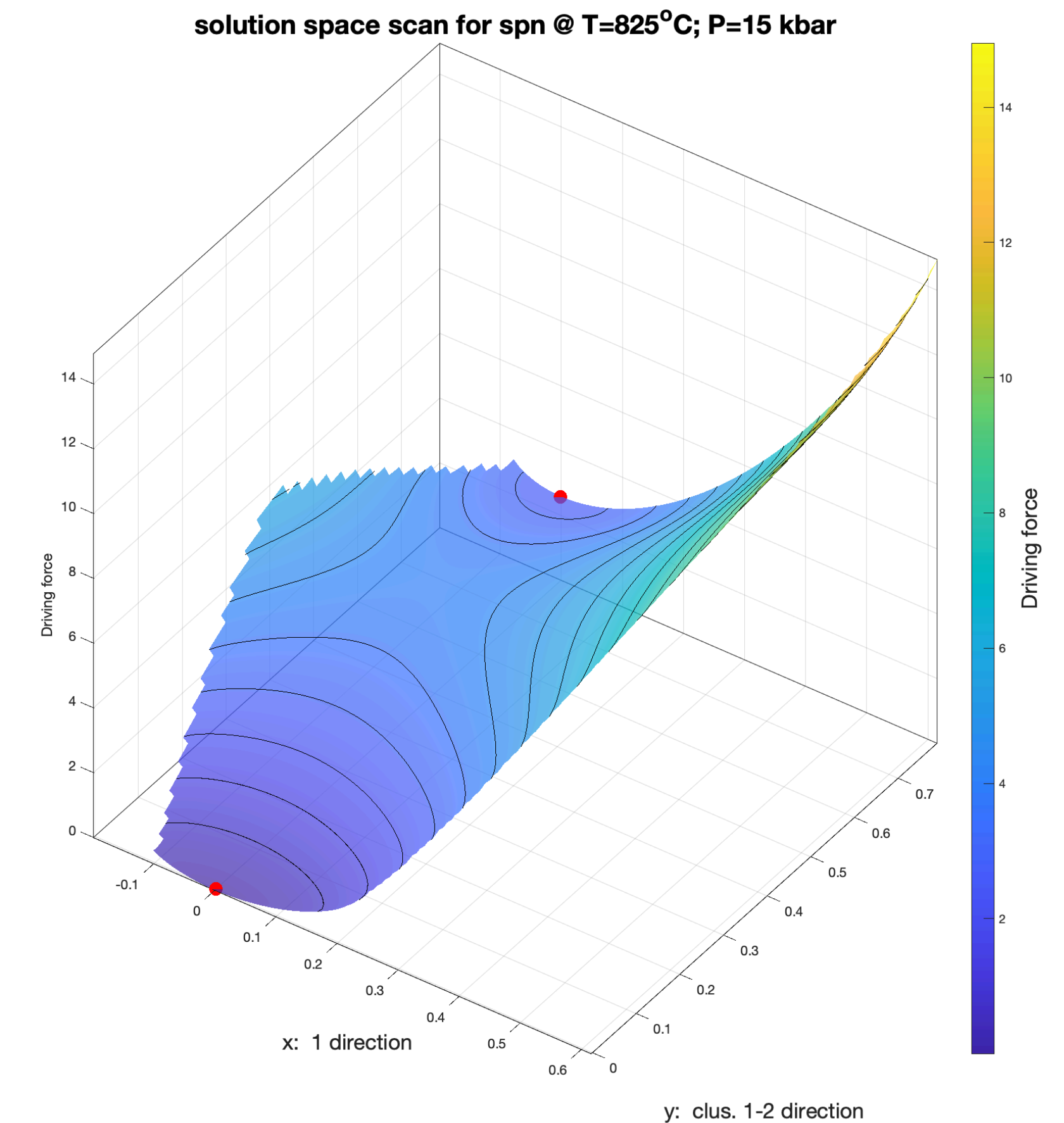
- For KLB1, in nearly all cases single minimum
 - If a second one occurs, it is often inadmissible
 - Complexities in solving this come from (nonlinear) constraints
- **Gradient-based approaches should work reasonably well**



2nd (more stable) solution for SPN, but not allowed because of constraints



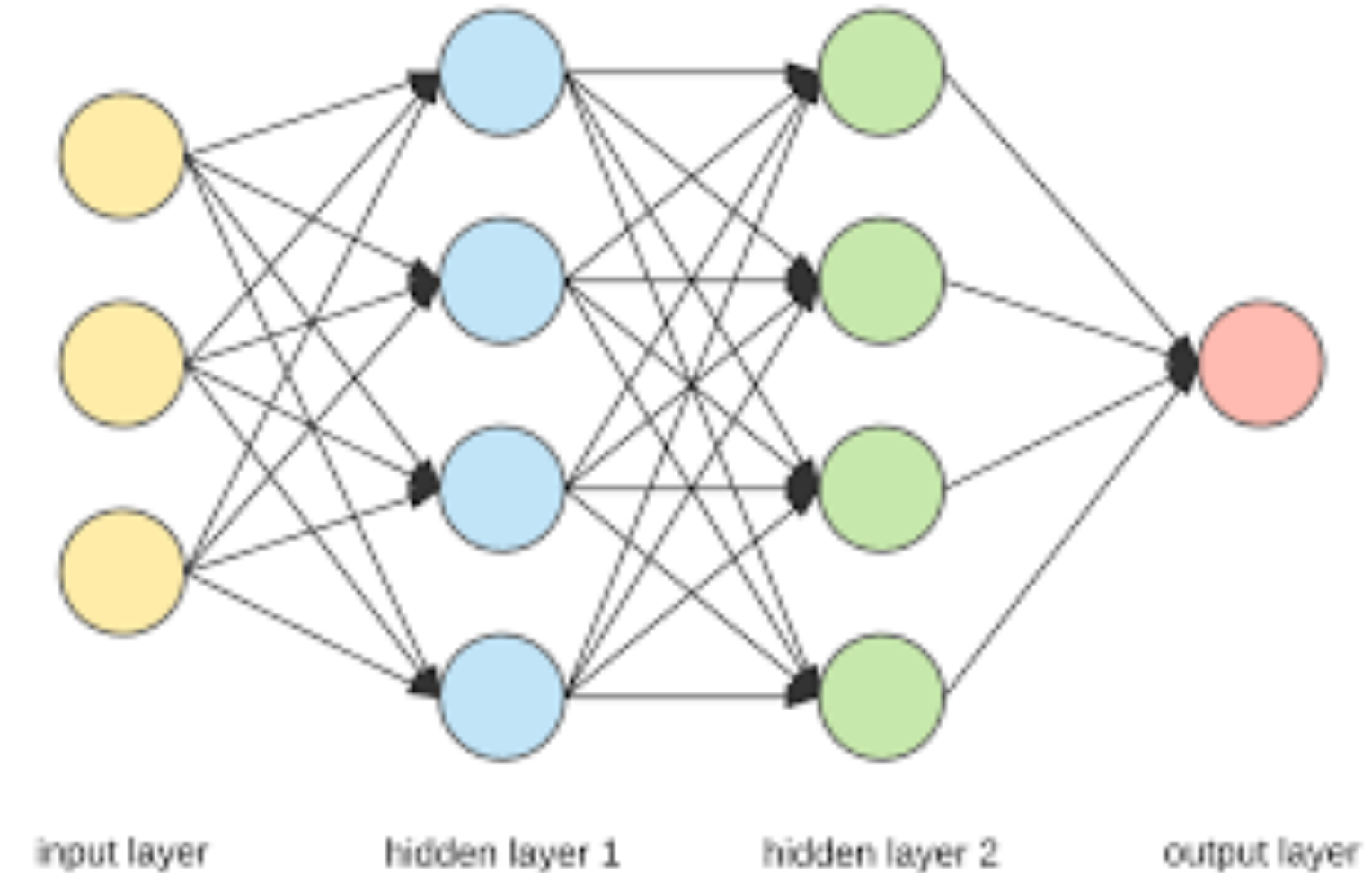
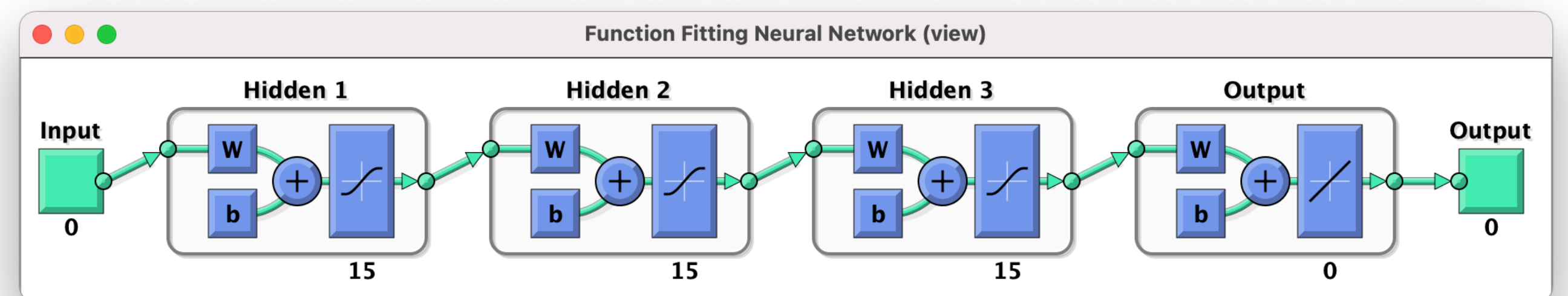
Example with 2 minima



- Here, local optimisers may get trapped in the wrong minima

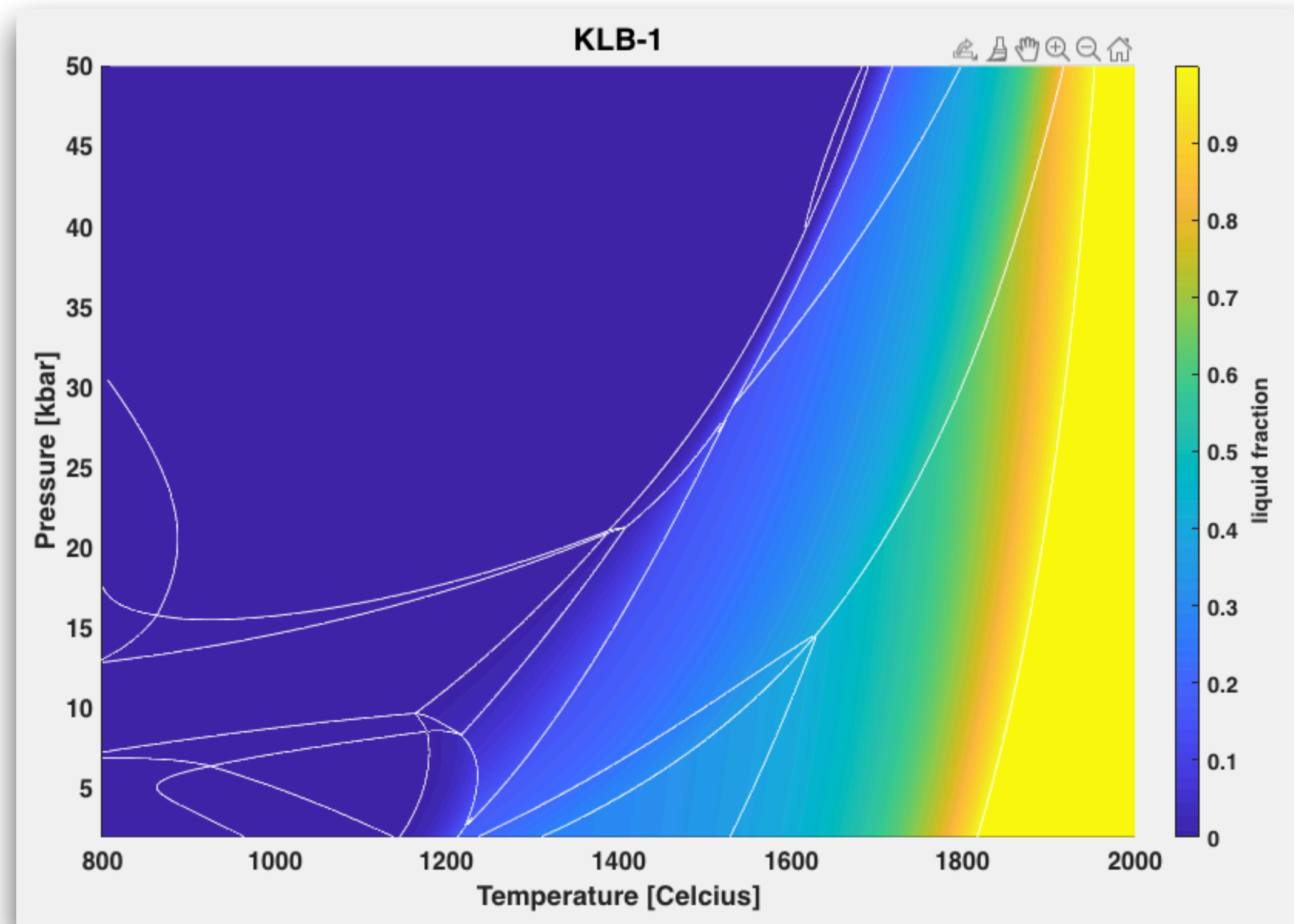
Neural networks

- Basically “fitting” tool to nonlinear functions.
- 1 or 3 layer model:
 - Input: P & T (2D)
 - Output: Fraction of stable assemblages (here 11D)
 - Trained with ~9k data points

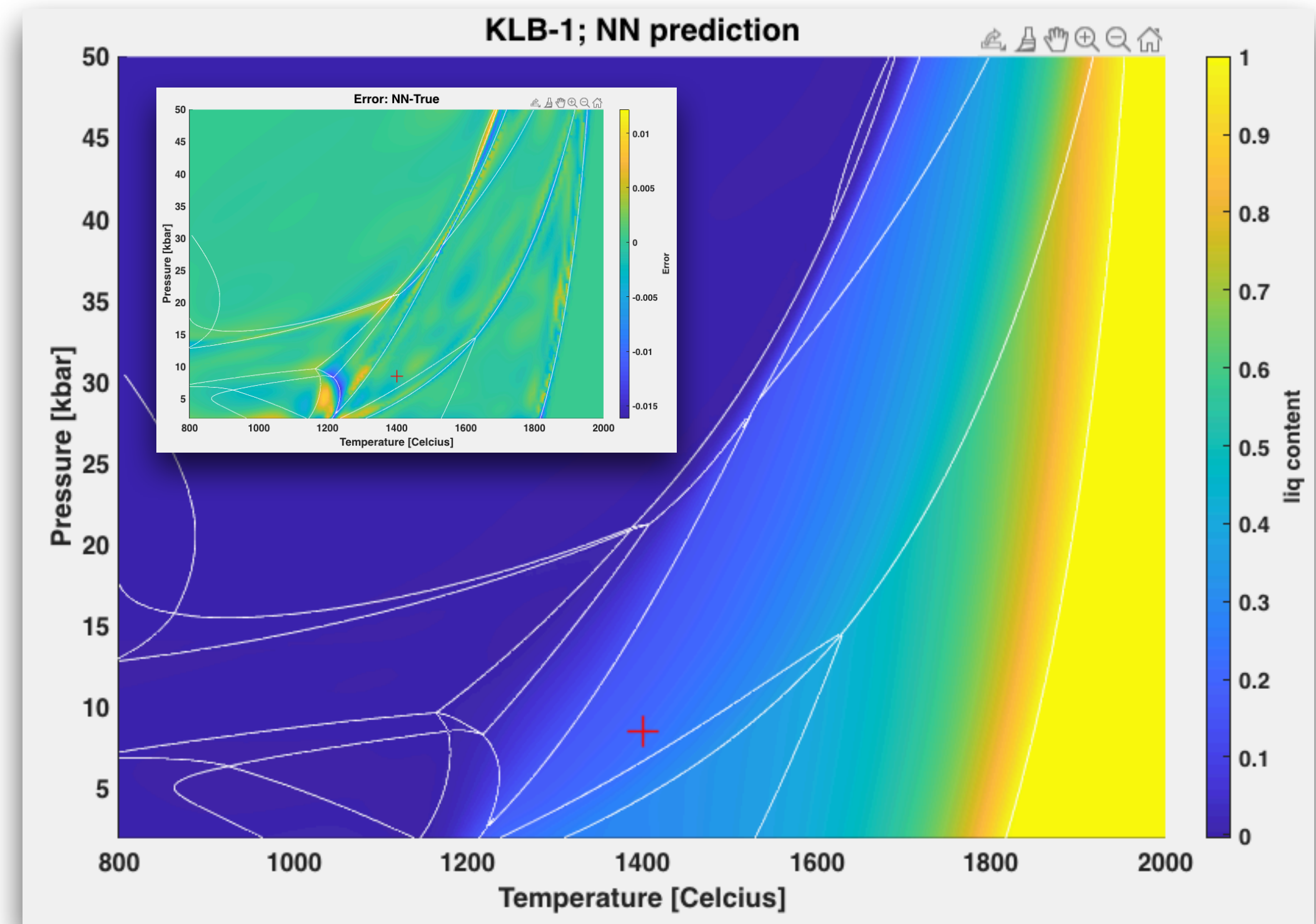


Example - melt content

True solution



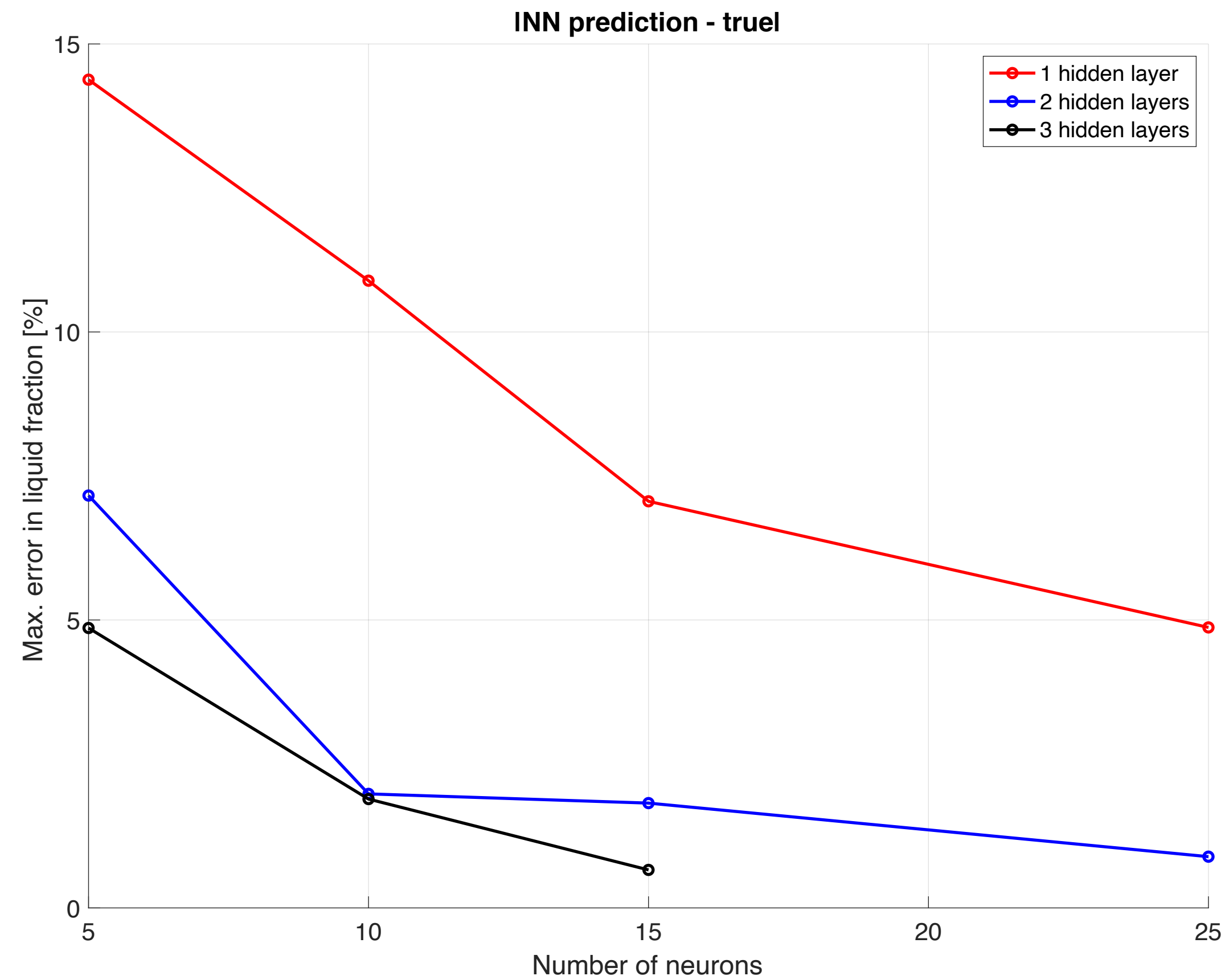
Trained NN (3 layers)



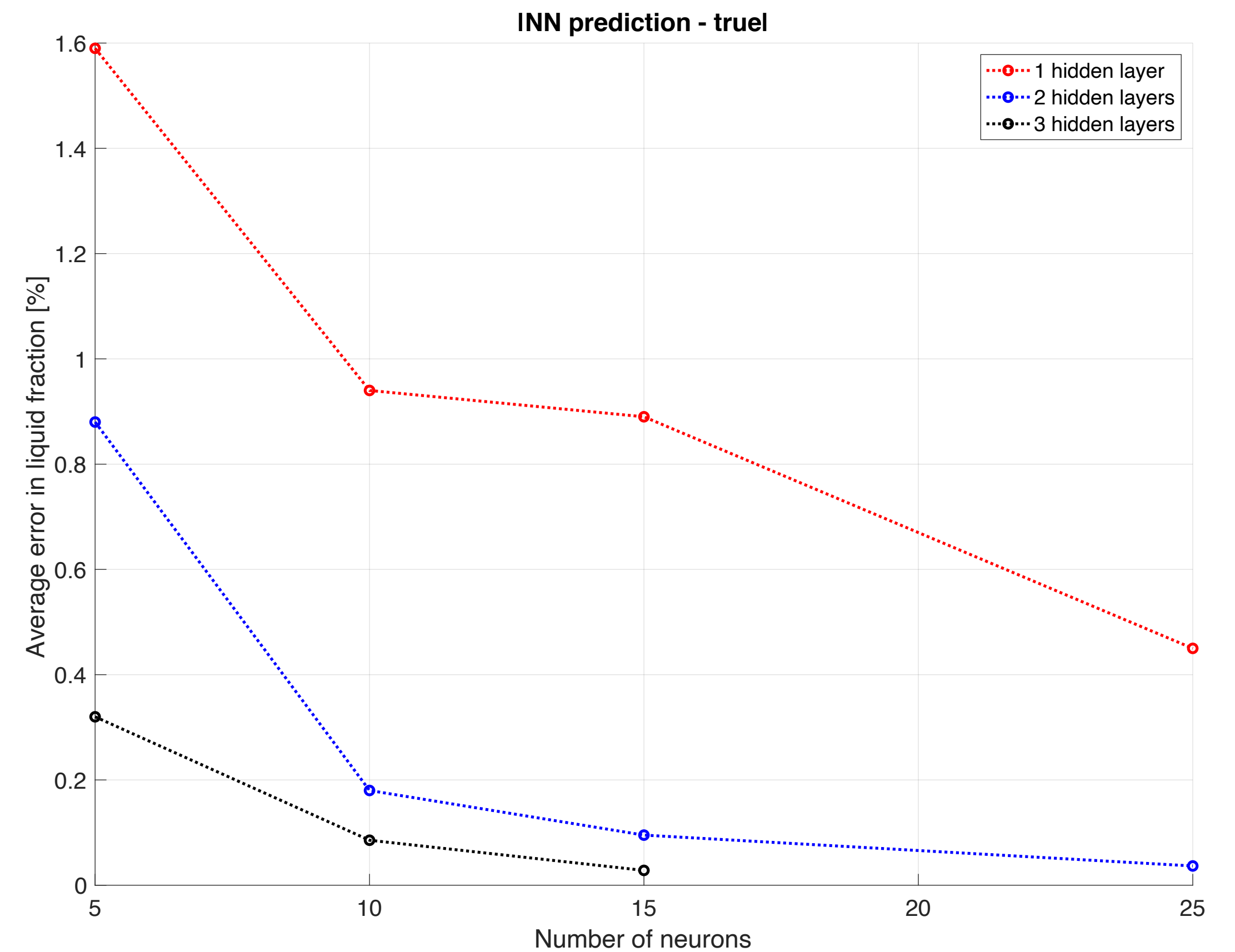
- NN does a very good job at predicting melt content

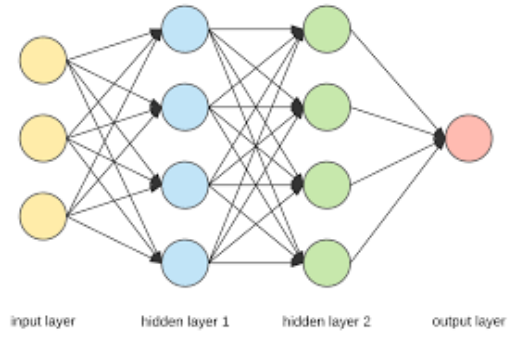
Error: systematics

Maximum error



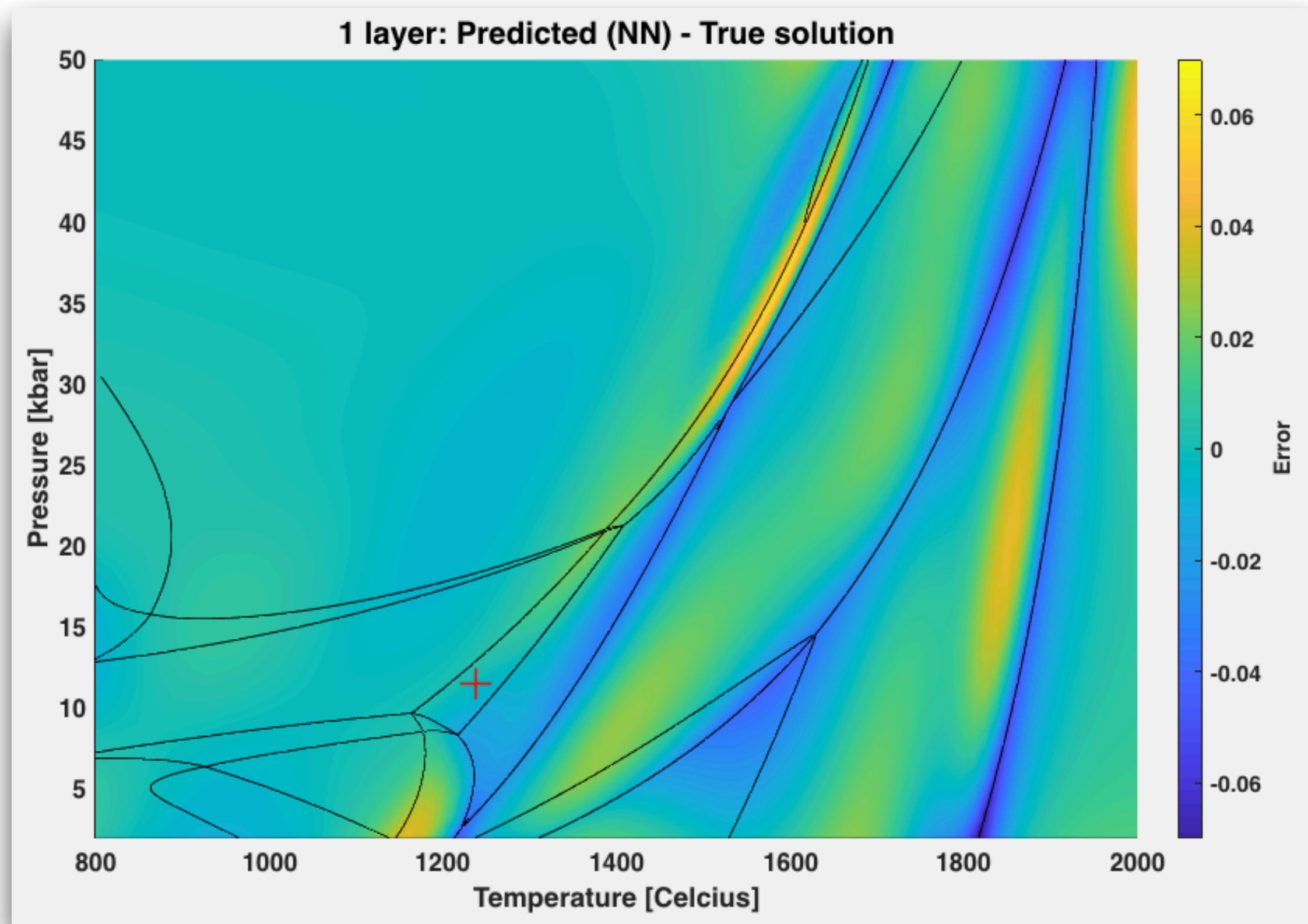
Average error



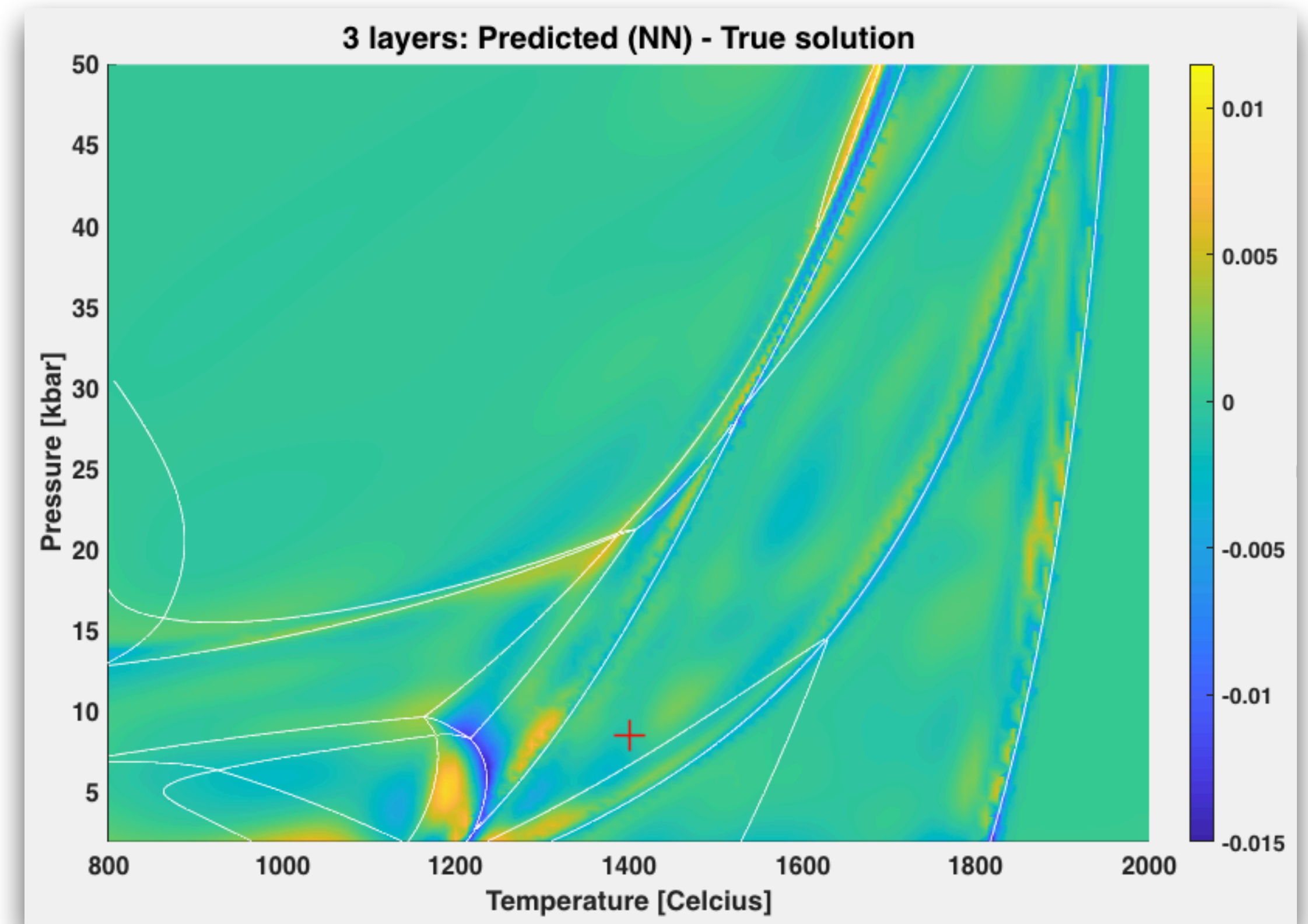


Error vs. # of layers

1 layer/15 neurons per layer



3 layers/15 neurons per layer

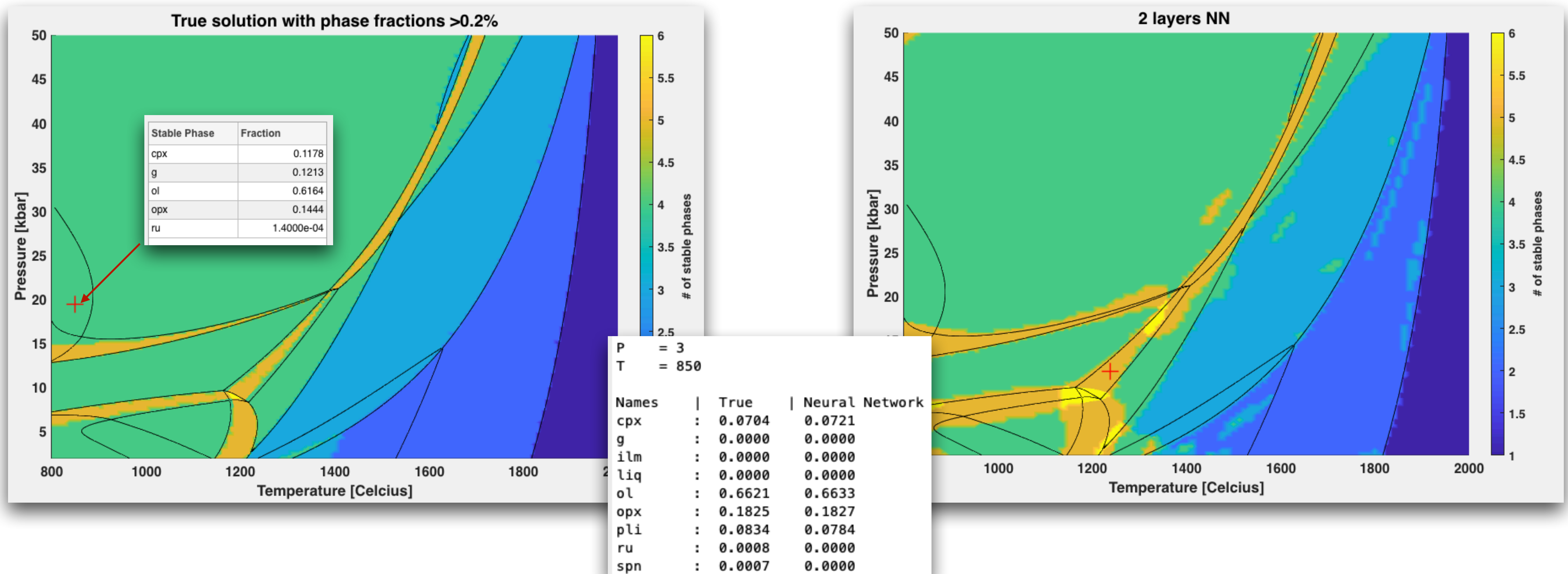


- More layers help (but beware of overfitting if you use too many!)

What about predicting the full diagram?

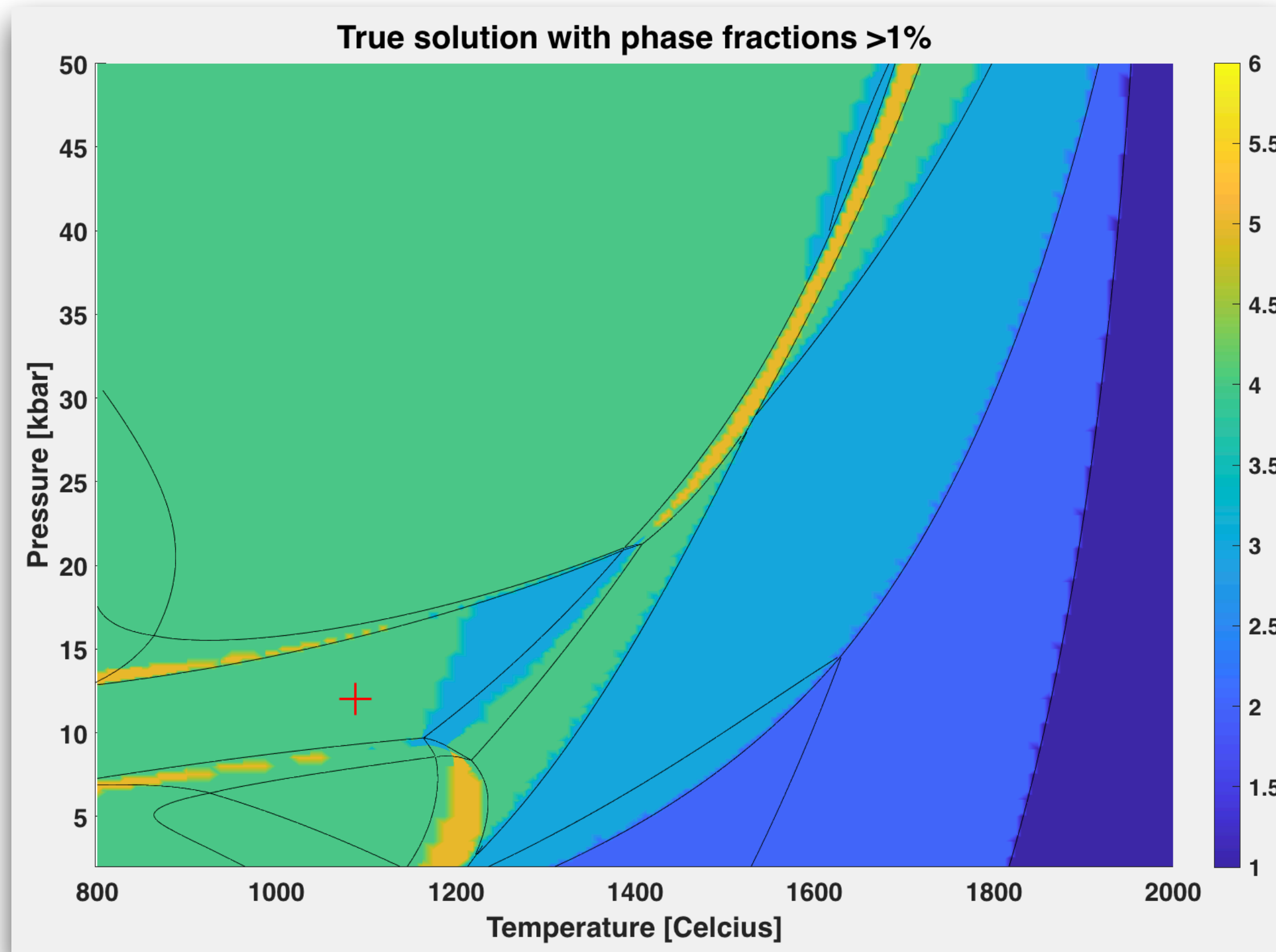
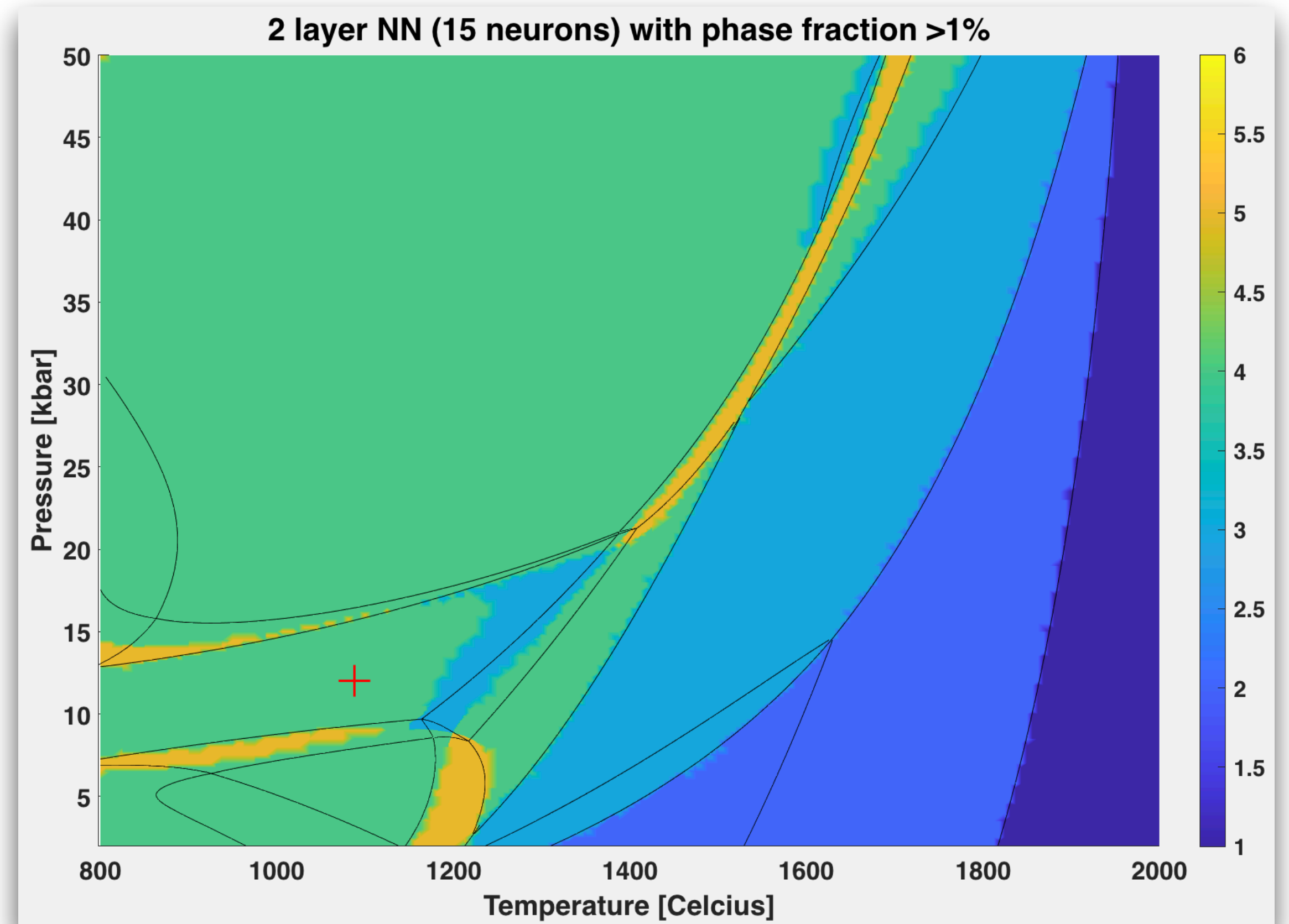
True solution (~few minutes)

Predicted (~0.1 seconds)



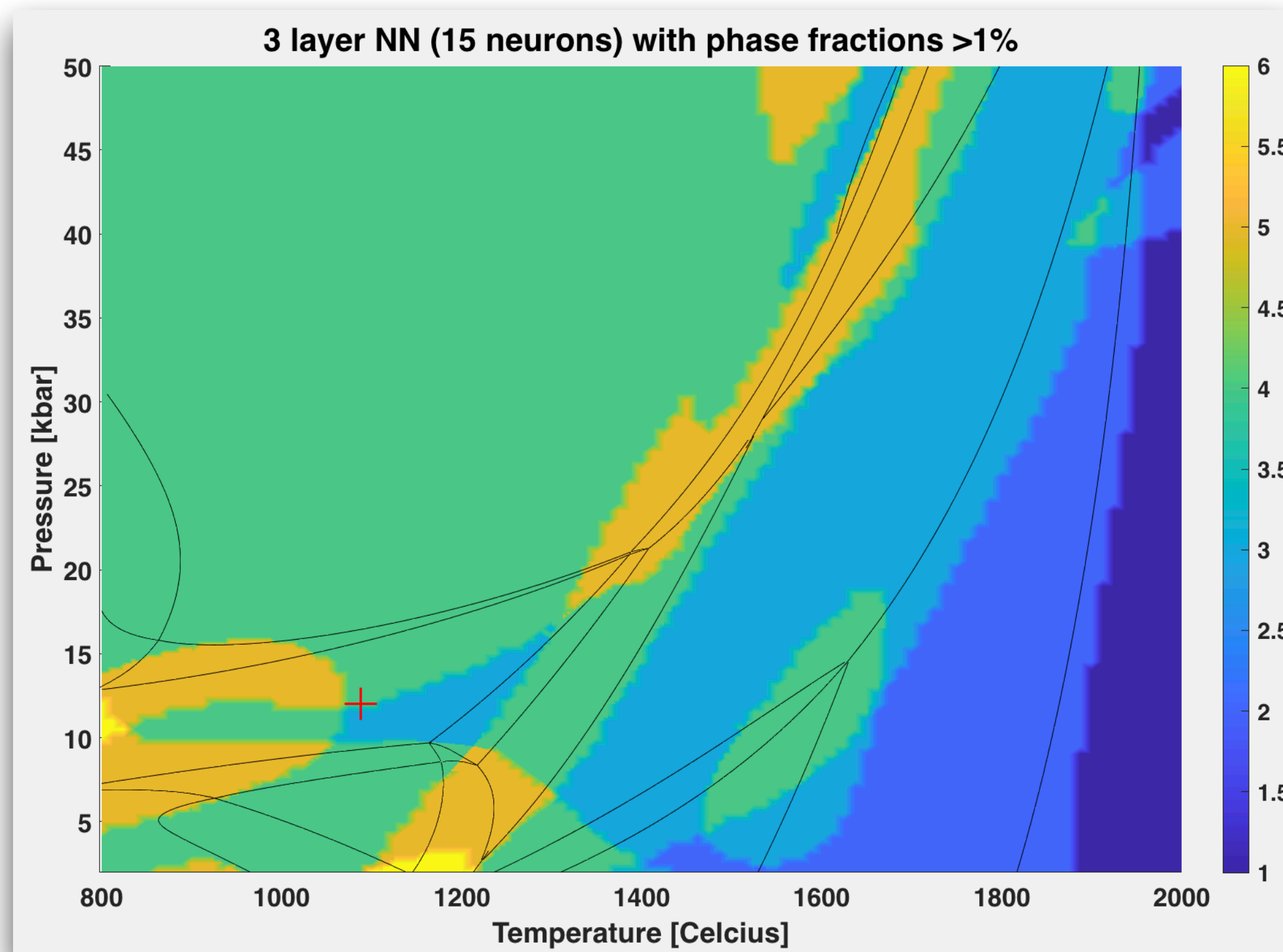
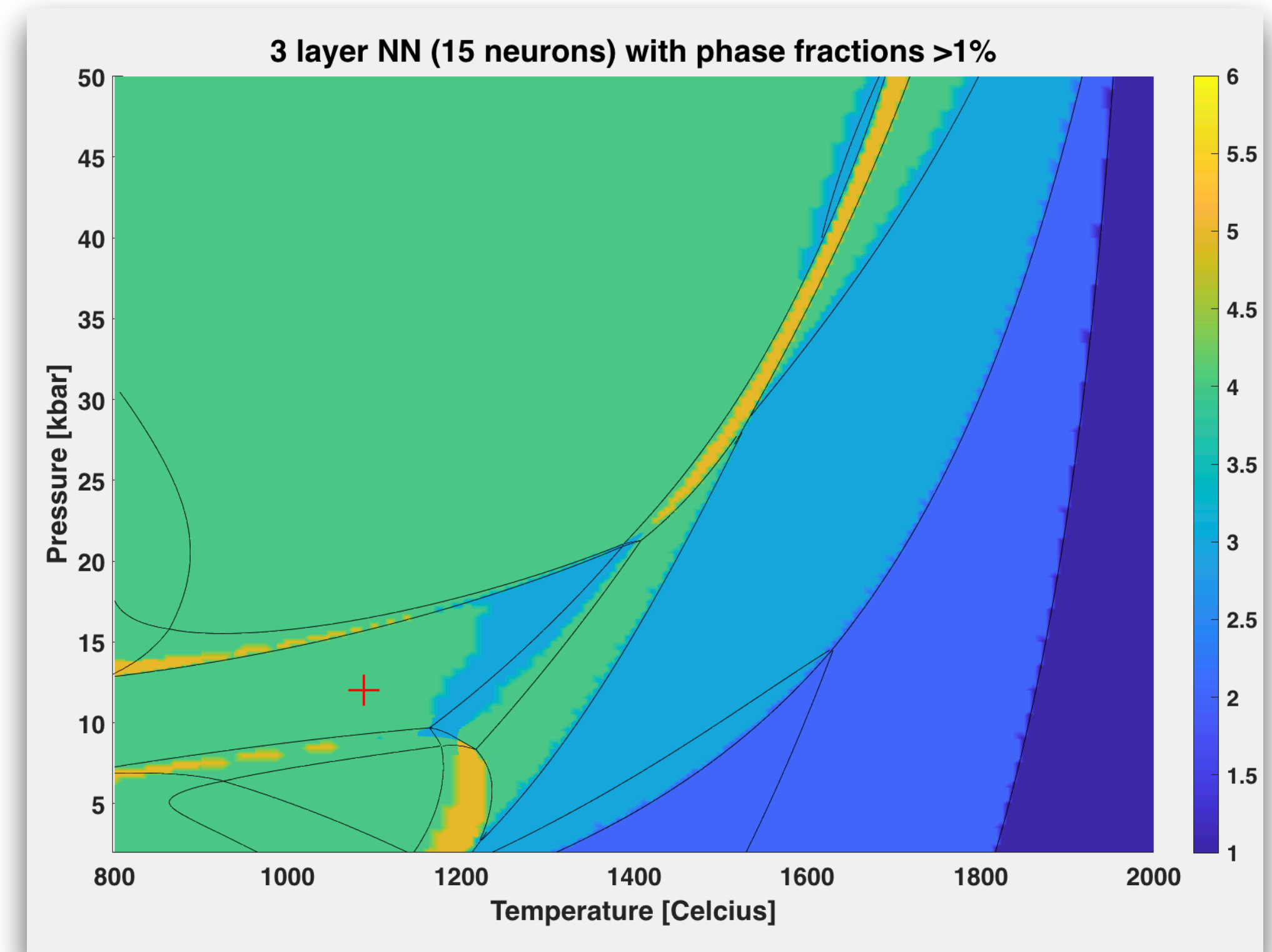
- ▶ Not great; largest differences in fields with small fractions
- ▶ Yet, we can also estimate the chemistry for every field

Mass fraction $> 0.1\%$



- Main fields are captured better

Effect of # of layers

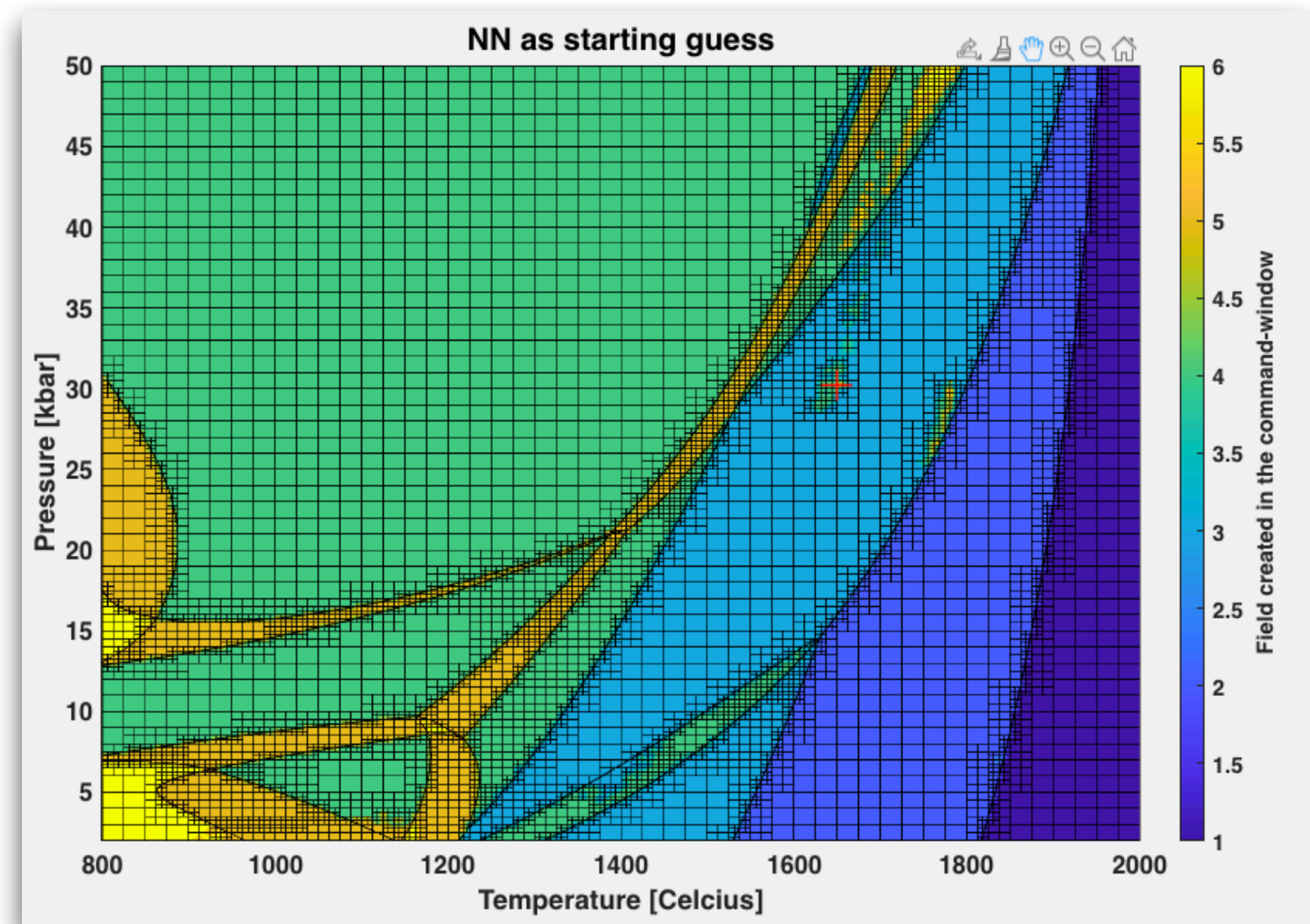


- Having >2 layers seems to work best

Use NN as initial guess

3 layers NN

- Use NN to estimate the initial composition of solid solutions
 - Examples:
 - olivine [4 end members]
 - spinel [8 end members]
 - clinopyroxene [10 end members]
 - melt [12 end members]
- Employ this as starting guess (rather than default values we use)



Solution is less good than without initial guess
Not fully clear yet why (*work in progress*)

Summary

- New thermodynamics code (under development)
- Local minima
 - G surfaces typically smooth
 - Computational challenges from (nonlinear) inequality constraints
- Neural networks
 - Quite good approximations of phase fractions
 - Computational challenges from (nonlinear) inequality conditions
- To be done
 - Incorporate H₂O-rich compositions
 - Train NN with variable chemistry as well
 - **Physics Informed Neural Networks (PINN)**

