PX915-A Specification

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General Targets

- This project will use the phase field model of spinoidal decomposition to simulate a binary alloy.
- The software will include a solver that will solve the 2D Cahn-Hilliard equations and calculate various parameters about the alloy, with parameters from an input file.
- The software will include visualisation of the solution and will record the data at each time step.
- Documentation of the software will be included. Documentation will be composed of installation and usage instructions.
- Version 1 of this software will be completed by Thursday 26th May 2022.

Specific Features

- The following attributes of the alloy will be calculated:
  - Bulk free energy density
  - Bulk chemical potential
  - Total chemical potential (inclusive of interfacial effects)
- The software will be hosted as open-source on Github using the GNU General Public License v3.0.
- The software will be written to run on x86-64 shared-memory architectures.
- The user will be able to input a file containing the input parameters for the solver.
- The Cahn-Hilliard equations will be solved using a finite-difference method.
- Visualisation of the solution will consist of animations over the specified time interval, as well as plots of quantities, such as the RDF.
- The code will be validated by comparing the visualised steady-state (i.e. final concentration field) for simple starting conditions (e.g. constant, uniform 50/50 split, or a step-like concentration field), for which steady-state solutions can be readily predicted from spinodal decomposition theory.
- Error handling will be built in to the software, which will include validation of user-specified parameters.
- The alloy will be modelled on a 2D grid with periodic boundary conditions.
- The solver will be written in Modern Fortran (2008 standard), the visualisation will be written in Python 3 and installation scripts will be written in bash/Make.
- The software will be parallelised to scale on multiple cores, and be operable on both shared and non-shared memory architecture.
- The solver will include a checkpoint system to allow the user to continue from a run stopped prior to completion.