Verification and Validation in Scientific Computing Project

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This project report describes a verification and validation study of the Allen–Cahn reaction-diffusion PDE. The source code used is available at `https://github.com/Steven-Roberts/VVSC-Project`.

I. Introduction

The Allen–Cahn equation is a reaction-diffusion partial differential equation (PDE) used to model phase separation for alloy systems and is governed by

$$\begin{aligned} \frac{\partial u}{\partial t} &= \alpha \nabla^2 u + \beta f(u) + S && \text{in} \quad \Omega \times [0, T], \\ \frac{\partial u}{\partial \vec{n}} &= 0 && \text{in} \quad \partial\Omega \times [0, T], \\ u &= u_0 && \text{in} \quad \Omega \times \{0\}. \end{aligned} \tag{1}$$

In [1], where this model was originally proposed, the authors model the motion of antiphase boundaries in an Fe-Al alloy. The Allen–Cahn equation can also be viewed as L^2 gradient flow of the Ginzburg–Landau free energy functional [2].

The model parameter $\alpha = M\varepsilon^2$, where M is the "mobility" and ε is the distance separating the boundary surfaces. Mobility is a positive constant relating the interfacial velocity to thermodynamic driving force [1]. The reaction term $f(u)$ is the derivative of a double-well potential. We have included an additional source term $S(x, y)$ to easily support order verification studies using the method of manufactured solutions. The system response quantity (SRQ) that we consider is the average solution value at the final time:

$$\text{SRQ} = \frac{1}{\text{Area}(\Omega)} \int_\Omega u(T, x) \, \mathrm{d}x \, .$$

In this work, we consider the 2D spatial domain $\Omega = [0, 1] \times [0, 1]$ and timespan $[0, 1]$. The spatial domain is discretized using second order, central finite differences with homogeneous Neumann boundary conditions. Each mesh cell is of size $\Delta x \times \Delta x$. In time, a second order Rosenbrock method is used with the fixed timestep Δt.

There are two MATLAB software packages used to implement the numerical experiments performed in this study. The first, ODE Test Problems, provides a semi-discretization of eq. (1) in space and the Jacobian matrix for the system of ordinary differential equations (ODEs). The second package, MATLODE, offers a second order Rosenbrock time discretization method among many others.

II. Code verification

In order verify the correctness of this MATLAB implementation of the Allen–Cahn problem, a convergence test was conducted to see if the theoretically predicted order of convergence can be achieved. In order to exactly compute errors in the convergence study, the method of manufactured solution was used to generate a source term S such that a simple, closed form solution u exists. In particular, the parameters were fixed at $\alpha = \beta = 1$, and the exaction solution was selected to be

$$u(t, x, y) = e^{-t} \left(\cos(2\pi x) + \cos^2(4\pi y) \right), \tag{2}$$

which is compatible with the Neumann boundary conditions. Substituting this into eq. (1) and solving for the unknown source term yields

$$S(t, x, y) = e^{-3t} \left(e^{2t} \left(\left(4\pi^2 - 2 \right) \cos(2\pi x) + \left(32\pi^2 - 1 \right) \cos(8\pi y) - 1 \right) + \left(\cos(2\pi x) + \cos^2(4\pi y) \right)^3 \right).$$

Suppose u^F is the numerical solution on at time $T = 1$ at all grid points, but flattened out so as to form a vector of dimension d. Let u^{ex} be the exact solution at time $T = 1$, similarly flatten into a vector. The following three norms were

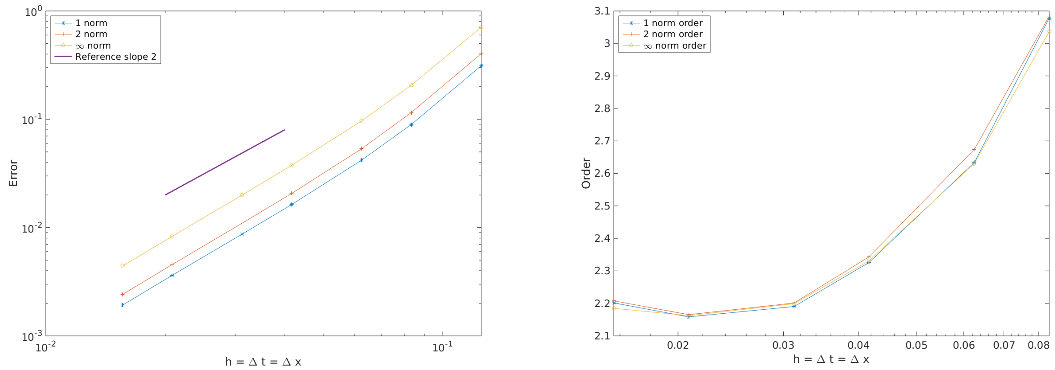


Fig. 1 Error and order of convergence as the spatial and temporal meshes are simultaneously refined.

used to measure the error between the exact and numerical solutions:

$$\|x\|_1 = \frac{1}{d}\sum_{i=1}^{d}\left|u_i^F - u_i^{\mathrm{ex}}\right|$$

$$\|x\|_2 = \sqrt{\frac{1}{d}\sum_{i=1}^{d}\left|u_i^F - u_i^{\mathrm{ex}}\right|}$$

$$\|x\|_\infty = \max_i \left|u_i^F - u_i^{\mathrm{ex}}\right|.$$

As there is both spatial and temporal convergence to be considered, we define a single discretization parameter $h = \Delta x = \Delta t$. As $h \to 0$, we expect second order convergence.

Figure 1 presents the results of the convergence test. We can see the order of convergence is slightly higher than two, but this result is still consistent with the theoretical order, which serves as a lower bound. It is possible the simple exact solution eq. (2) causes certain derivative in the Taylor series expansion of the error to vanish.

We note this test is a necessary condition for code verification but certainly not sufficient. Using uniform timesteps is the most sensible way to perform the convergence test, but it means the adaptive timestepping part of the integrator in the model is not tested. Moreover, we only considered the case when $\alpha = \beta = 1$. A more thorough and convincing test could include manufactured solutions for several parameter values. Otherwise, the manufactured solution test provides full verification of the Allen–Cahn code.

III. Solution verification

IV. Extrapolation of model form uncertainty

In this section we consider extrapolating the area validation metric (AVM) to estimate model form uncertainties outside the range of α parameters used in the numerical experiments. The parameter β is assume to be normally distributed with mean 1.25 and standard deviation 0.5. In previous experiments conducted in homework 5, α was fixed at 1, but now we are interested in the AVM when $\alpha = 2.5$.

α	1	1.1	1.35	1.42	1.59	1.7	1.88	1.9	1.92	2.1
AVM	0.0788	0.0801	0.0955	0.0922	0.100	0.109	0.132	0.130	0.148	0.155

Table 1 Validation metrics for several values of α. The first column of data comes from homework 5, while the others are randomly generated.

Using the data presented in table 1, a least squares linear fit was used to approximate the AVM for different values of α. This is presented graphically in fig. 2 along with a 95% prediction interval. When $\alpha = 2.5$, we can see the extrapolated AVM is approximately 0.176. The corresponding 95% prediction interval is $[0.1490, 0.2030]$.

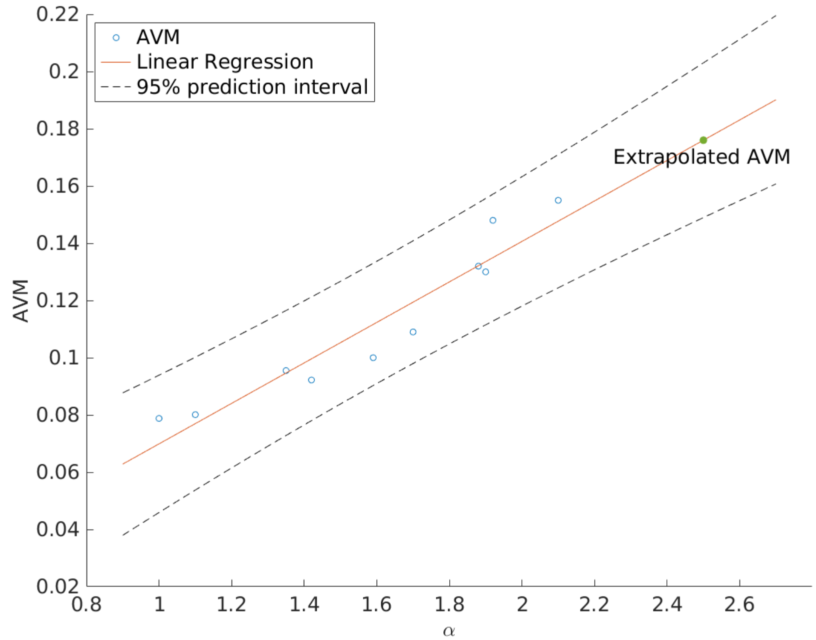


Fig. 2 Linear regression of data from table 1 and 95% prediction interval.

V. Uncertainty propagation

Consider a scenario where the model parameter β is normally distributed with mean 1.25 and standard deviation 0.5 and α is an epistemic uncertainty in the interval $[0.1, 1]$. In this section, we consider the propagation of these two uncertainties through the model and their effect on the SRQ. A nested sampling procedure is to produce a p-box approximating the upper and lower bounds of the cumulative distribution function of the SRQ. In the experiment, Latin hypercube sampling with 25 samples was used to sample β, while α was selected to be evenly spaced values in the uncertainty interval with 5, 25, and 50 samples. Also, we select the discretization parameters as $\Delta x = \Delta t = \frac{1}{64}$.

Figure 3 plots the results of this experiment. Inside the p-boxes are all the sample CDFs for each value of α from the evenly spaced epistemic sample points, as well as the CDF from treating α as a uniform random variable over $[0.1, 1]$. We note that treating the interval as a uniform distribution may not be an accurate or realistic assumption. Varying the number of epistemic samples had little effect on the p-box, but does show more clearly the distribution of samples within the p-box. These samples and the probabilistic CDF are distributed closer to the right side of the p-box.

VI. Estimating numerical uncertainties

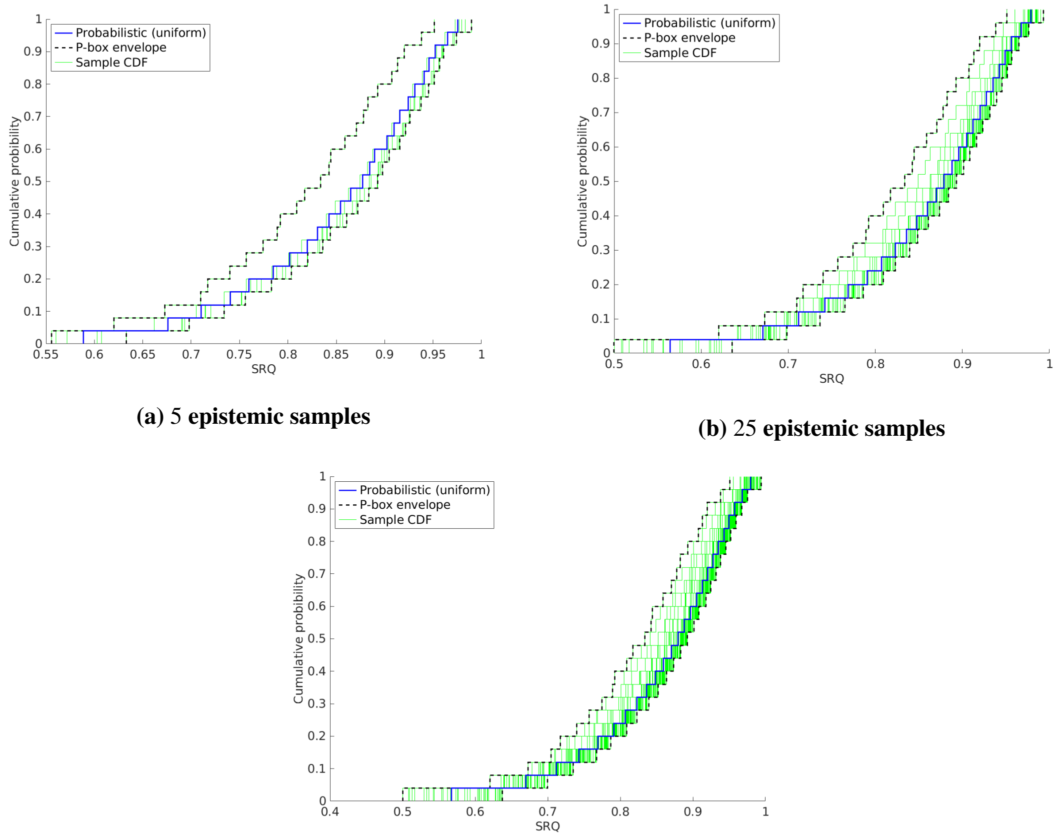
To measure the numerical uncertainties, in particular discretization errors, the Grid Convergence Index (GCI) was used:

$$GCI = \frac{F_s}{r^p - 1}|f_2 - f_1|.$$

Here f_1 and f_2 are the SRQs computed using $\Delta x = \Delta t = \frac{1}{64}$ and $\Delta x = \Delta t = \frac{1}{128}$, respectively. The order is $p = 2$, the ratio of mesh sizes if $r = 2$, and F_s is a safety factor. As only two numerical different discretizations were used, the safety factor was set to the conservative value of 3.

The GCI will vary with the model parameters, so we consider four extreme cases to estimate an upper bound of the GCI for relevant test cases. For the parameter α, which is assumed to be an epistemic uncertainty, we consider the interval endpoints $\alpha = 0.1, 1$. As we have assumed β is normally distributed, we consider the GCI when β is two standard deviations above and below the mean.

Table 2 lists the GCI for the four corner cases. The largest value is 1.01×10^{-4}, which is quite small relative to other uncertainties discuss in this report.



(a) 5 **epistemic samples**

(b) 25 **epistemic samples**

(c) 50 **epistemic samples**

Fig. 3 Input uncertainty propagated to the SRQ represented as a p-box

α	β	GCI
0.1	0.25	5.42×10^{-5}
0.1	2.25	1.94×10^{-6}
1	0.25	1.01×10^{-4}
1	2.25	7.71×10^{-5}

Table 2 GCI for four model parameter scenarios

I was unable to quantify round off error due to the inability to run experiments in single precision. Iterative error is not relevant as direct linear solvers are used by the Rosenbrock method.

VII. Total prediction uncertainty

Figure 4 presents the total prediction uncertainty. Most of it comes from model form uncertainty followed by input uncertainty. Numerical uncertainty contributes relatively little as it are orders of magnitude smaller than the others. In fact, in fig. 4, the numerical and model uncertainty lines essentially overlap.

Based on these results, the most sensible way to reduce uncertainty in this to reduce model form uncertainty. This could involve choosing a different model, adding missing or ignored model dynamics, and identifying model biases.

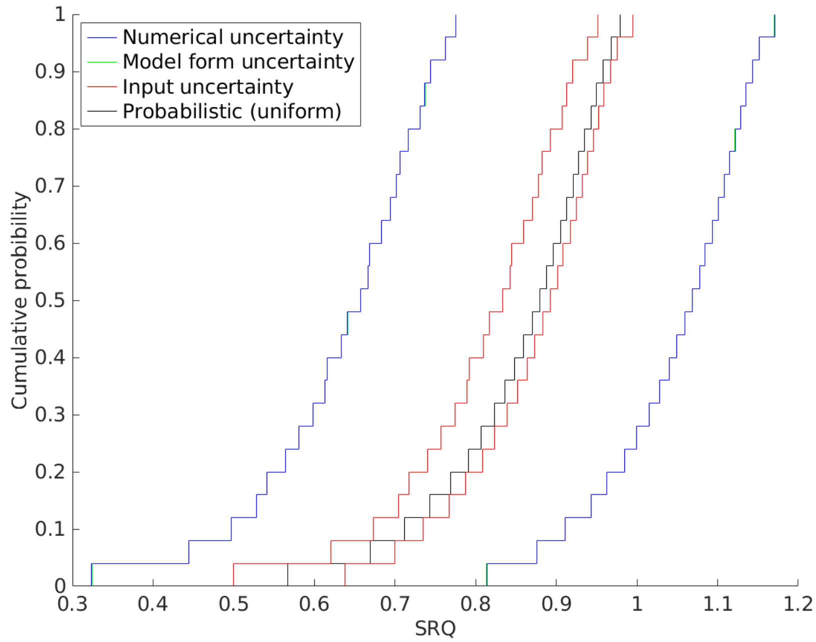


Fig. 4 Total prediction uncertainty. Note the lines for the numerical and model form nearly overlap.

VIII. Conclusion

The experimental results from the Allen–Cahn PDE are influenced by many factors including discretization errors, model input uncertainties, and model biases. In this report we explore and present estimates of the uncertainties and their effect on a system response quantity of interest. In order to reduce the uncertainties, it is recommended to focus on model form uncertainties. Moreoever, the discretization errors are small enough that coarser spatial and temporal meshes are possible, speeding up the experiments.

References

[1] Allen, S. M., and Cahn, J. W., "A microscopic theory for antiphase boundary motion and its application to antiphase domain coarsening," *Acta metallurgica*, Vol. 27, No. 6, 1979, pp. 1085–1095.

[2] Feng, X., and Prohl, A., "Numerical analysis of the Allen–Cahn equation and approximation for mean curvature flows," *Numerische Mathematik*, Vol. 94, No. 1, 2003, pp. 33–65.