In this notebook the relations for the basic phase-field relations are derived as well as the eigenvalue estimates using Gershgorin's circle theorem.

First, we define the free energy from which the eventual PDEs will be derived.

$$F = \int \left(\sum_{\alpha=0}^{N-1} g(\alpha, c_i(c)) h(\alpha, \phi_a) + \sum_{\substack{\alpha+1 \leq \beta \leq N-1 \\ 0 \leq \alpha \leq N-1}} \left(-A_{\alpha,\beta} \nabla \phi_\alpha \nabla \phi_\beta + B_{\alpha,\beta} \phi_\alpha \phi_\beta \right) \right) dx$$

After appropriate simplification for the variational derivative of F wrt. ϕ using the two-phase simplification ($\phi_\beta = 1 - \phi_\alpha$) we get an ODE for the equilibrium state, from which A, B can be related to W, γ.

False

$$W = \frac{\sqrt{A_{\alpha,\beta}}}{\sqrt{B_{\alpha,\beta}}}$$

$$\gamma = \frac{\pi \sqrt{A_{\alpha,\beta}} \sqrt{B_{\alpha,\beta}}}{4}$$

Inverting the W, γ solution gives us the expressions for A, B:

$$A_{\alpha,\beta} = \frac{4W\gamma}{\pi}$$

$$B_{\alpha,\beta} = \frac{4\gamma}{\pi W}$$

For the mobility we form the one-phase evolution while formally applying Steinbach's ansatz.

$$\frac{\delta F}{\delta \phi_\alpha} = -\left(\phi_\alpha(x,t) - 1\right) B_{0,1} - \phi_\alpha(x,t) B_{0,1} - 2 \frac{\partial^2}{\partial x^2} \phi_\alpha(x,t) A_{0,1}$$

$$\frac{\partial}{\partial t} \phi_\alpha(x,t) = \frac{L \left(2\phi_\alpha(x,t) B_{0,1} + 2 \frac{\partial^2}{\partial x^2} \phi_\alpha(x,t) A_{0,1} - B_{0,1} \right)}{2}$$

Next we transform the variational derivative from the Cartesian to the local coordinate system (LCS), with r normal to the interface and a number of tangential vectors t_n appropriate for the dimension; though we don't use the latter here.

$$\frac{\partial}{\partial t}\phi_\alpha(r,t) = \frac{L\left(2\left(\kappa\frac{\partial}{\partial r}\phi_\alpha(r,t) + \frac{\partial^2}{\partial r^2}\phi_\alpha(r,t)\right)A_{0,1} + 2\phi_\alpha(r,t)B_{0,1} - B_{0,1}\right)}{2}$$

Assuming that this basically causes the phase-field to move its equilibrium profile at some velocity, we can subtract out the equilibrium part; see e.g. doi.org/10.1103/PhysRevB.78.024113 for further justification of this assumption in the limit of $W \ll R, R \approx \frac{1}{\kappa}$.

$$\frac{\partial}{\partial t}\phi_\alpha(r,t) = L\kappa\frac{\partial}{\partial r}\phi_\alpha(r,t)A_{0,1}$$

Next, we define the phase-field velocity as $\frac{\partial\phi_\alpha}{\partial t}\left(\frac{\partial\phi_\alpha}{\partial x}\right)^{-1}$ and compare it with the mean curvature flow interface velocity to obtain L:

$$v = M\gamma\kappa$$

$$v_{pf} = L\kappa A_{0,1}$$

$$L = \frac{\pi M}{4W}$$

Next, we estimate the eigenvalues for a two-phase system. This requires a bit of setup so we can apply Gershgorin's circle theorem on effectively a single row of the discretized RHS. We assume this row to be the "worst case", i.e. containing the largest coefficients.

The full KKS RHS with inequal k and not using the two-phase simplifcation is horribly long and nonlinear. We make use of the simplifications to get something we can reason about to account for overestimates. It actually breaks the automated display here, but you get the idea.

$$\frac{\partial}{\partial t} c_A(x,t) = \frac{D \Bigg(\Bigg(- \Big(\left(\left(\phi_0(x) - 1 \right) k_v - \phi_0(x) k_s \right) \left(\frac{d}{dx} \phi_0(x) c_{0_s} k_s - \frac{d}{dx} \phi_0(x) c_{0_v} k_v + \frac{d}{dx} c_A(x) k_s \right) + \left(k_s - k_v \right) \left(\left(\phi_0(x) - 1 \right) c_{0_s} k_s - \left(\phi_0(x) - 1 \right) c_{0_v} k_v + c_A(x) k_s \right) \frac{d}{dx} \phi_0(x) \Big) \frac{d}{dx} \phi_1(x) - \Big(\left(\left(\phi_0(x) - 1 \right) k_v - \phi_0(x) k_s \right) \left(\frac{d}{dx} \phi_0(x) c_{0_s} k_s - \frac{d}{dx} \phi_0(x) c_{0_v} k_v + \frac{d}{dx} c_A(x) k_v \right) + \left(k_s - k_v \right) \left(\phi_0(x) c_{0_s} k_s - \phi_0(x) c_{0_v} k_v + c_A(x) k_v \right) \frac{d}{dx} \phi_0(x) \Big) \frac{d}{dx} \phi_0(x) \Bigg) \left(\left(\phi_0(x) - 1 \right) k_v - \phi_0(x) k_s \right) - \Bigg(\left(\left(\phi_0(x) - 1 \right) k_v - \phi_0(x) k_s \right)^2 \left(\frac{d^2}{dx^2} \phi_0(x) c_{0_s} k_s - \frac{d^2}{dx^2} \phi_0(x) c_{0_v} k_v + \frac{d^2}{dx^2} c_A(x) k_s \right) + \left(\left(\phi_0(x) - 1 \right) k_v - \phi_0(x) k_s \right) \left(k_s - k_v \right) \Bigg(\left(\phi_0(x) - 1 \right) \frac{d^2}{dx^2} \phi_0(x) c_{0_s} k_s - \left(\phi_0(x) - 1 \right) \frac{d^2}{dx^2} \phi_0(x) c_{0_v} k_v + c_A(x) \frac{d^2}{dx^2} \phi_0(x) k_s + 2 \left(\frac{d}{dx} \phi_0(x) \right)^2 c_{0_s} k_s - 2 \left(\frac{d}{dx} \phi_0(x) \right)^2 c_{0_v} k_v + 2 \frac{d}{dx} \phi_0(x) \frac{d}{dx} c_A(x) k_s \Bigg) + 2 (k_s - k_v)^2 \left(\left(\phi_0(x) - 1 \right) c_{0_s} k_s - \left(\phi_0(x) - 1 \right) c_{0_v} k_v + c_A(x) k_s \right) \left(\left(\frac{d}{dx} \phi_0(x) \right)^2 \right) \Bigg) \phi_1(x) - \Bigg(\left(\left(\phi_0(x) - 1 \right) k_v - \phi_0(x) k_s \right)^2 \left(\frac{d^2}{dx^2} \phi_0(x) c_{0_s} k_s - \frac{d^2}{dx^2} \phi_0(x) c_{0_v} k_v + \frac{d^2}{dx^2} c_A(x) k_v \right) + \left(\left(\phi_0(x) - 1 \right) k_v - \phi_0(x) k_s \right) \left(k_s - k_v \right) \Bigg(\phi_0(x) \frac{d^2}{dx^2} \phi_0(x) c_{0_s} k_s - \phi_0(x) \frac{d^2}{dx^2} \phi_0(x) c_{0_v} k_v + c_A(x) \frac{d^2}{dx^2} \phi_0(x) k_v + 2 \left(\frac{d}{dx} \phi_0(x) \right)^2 c_{0_s} k_s - 2 \left(\frac{d}{dx} \phi_0(x) \right)^2 c_{0_v} k_v + 2 \frac{d}{dx} \phi_0(x) \frac{d}{dx} c_A(x) k_v \Bigg) + 2 (k_s - k_v)^2 \left(\phi_0(x) c_{0_s} k_s - \phi_0(x) c_{0_v} k_v + c_A(x) k_v \right) \left(\left(\frac{d}{dx} \phi_0(x) \right)^2 \right) \Bigg) \phi_0(x) \Bigg)}{\left(\left(\phi_0(x) - 1 \right) k_v - \phi_0(x) k_s \right)^3}$$

After setting both k equal and using the two phase property, we get:

$$\frac{\partial}{\partial t} c_A(x,t) = D \frac{d^2}{dx^2} \phi_0(x) c_{0_s} - D \frac{d^2}{dx^2} \phi_0(x) c_{0_v} + D \frac{d^2}{dx^2} c_A(x)$$

The full RHS for the phase-field is similarly horrible; we only show it here after simplification.

$$\frac{\partial}{\partial t} \phi_0(x,t) = L \Big(2\phi_0(x) B_{0,1} - 5\phi_0(x) c_{00}^2 k_0 + 10\phi_0(x) c_{00} c_{01} k_0 - 5\phi_0(x) c_{01}^2 k_0 + 3 c_A(x) c_{00} k_0 - 3 c_A(x) c_{01} k_0 + 2 \frac{d^2}{dx^2} \phi_0(x) A_{0,1} - B_{0,1} + c_{00}^2 k_0 - 5 c_{00} c_{01} k_0 + 4 c_{01}^2 k_0 \Big)$$

First, to verify if the automated Gershgorin estimate here works, we apply it to the second-order central-difference discretization of a Laplacian $\nabla^2 c$, from which we recover the appropriate eigenvalues:

$$\lambda \leq 0 \wedge -\infty < \lambda$$

$$\lambda \geq -\frac{4}{dx^2}$$

Next we'll apply it to the KKS diffusion equation, yielding:

$$\lambda \leq \frac{4\left|Dc_{0_s} - Dc_{0_v}\right|}{dx^2}$$

$$\lambda \geq -\frac{4D}{dx^2} - \frac{4\left|Dc_{0_s} - Dc_{0_v}\right|}{dx^2}$$

Where we only care about the second one since its magnitude is larger than the former one.

This turns out to be an overestimate for the considered benchmarks. Generally $\lambda_c \approx -\frac{dD}{\Delta x^2}\left(4 + 2|c_{0,s} - c_{0,v}|\right)$ ($d =$ dimension) was employed, which yielded stable integration with the FEuler integrator, but increasing slightly above this bound showed instability. The usual diffusion bound is restricted further via an effective diffusivity $D|\Delta c_{eq}|$.

$$\lambda_c = -\frac{Dd\left(2\left|c_{0_s} - c_{0_v}\right| + 4\right)}{dx^2}$$

For the phase-field equation we obtain:

$$\lambda \leq 2LB_{0,1} - 5Lc_{0_0}^2 k_0 + 10Lc_{00}c_{01}k_0 - 5Lc_{0_1}^2 k_0 + \left|3Lc_{00}k_0 - 3Lc_{01}k_0\right| \wedge -\infty < \lambda$$

$$\lambda \geq 2LB_{0,1} - 5Lc_{0_0}^2 k_0 + 10Lc_{00}c_{01}k_0 - 5Lc_{0_1}^2 k_0 - \frac{8LA_{0,1}}{dx^2} - \left|3Lc_{00}k_0 - 3Lc_{01}k_0\right| \wedge \lambda < \infty$$

The estimate with the Δx^2 dependence (call it λ_1) should be absolutely larger than the one without. $\lambda_1 < 0$ holds ($A/dx^2 > B$ for reasonable choices of W, dx); λ_2's absolute value is bounded by $2LB + 3Lk|dc|$, compare to λ_1 with $A/dx^2 = B$, then one sees that $|\lambda_1| > |\lambda_2|$ and hence we only care about λ_1.

$$\frac{A_{\alpha,\beta}}{dx^2 B_{\alpha,\beta}} = \frac{W^2}{dx^2}$$

Again, this is an overestimate; stability was still achieved for

$$\lambda_\phi = \frac{L\left(-\frac{8dA}{dx^2} - \left(c_{0_s} - c_{0_v}\right)^2 k_0 - \left|c_{0_s} - c_{0_v}\right| k_0 + 2B\right)}{2}$$

As a side note, the phenomenon of "grid friction" in phase-field simulations, where the phase-field evolution is artificially slowed down in the limit of coarsely resolved interfaces, may be related to the ratio of $\frac{A}{dx^2 B}$ since it controls the sign of the largest eigenvalue, with smaller ratios of $\frac{W}{dx}$ (more coarsely resolved interface) leading to $B > A/dx^2$. Once the reaction term with B dominates and $\lambda_1 > 0$ the solution would blow up were it not for constraints on the ϕ values. This frustration between blow-up and the constraints may be the cause of grid friction. It might also be that just having some sufficiently large, positive eigenvalues causes this. It might be interesting to probe the discrete eigenvalues of some sharp phase-field models and whether they effectively force purely negative eigenvalues.

Finally, a note on how the speedup possibly varies with more or less accurate eigenvalue estimates, assuming they are still above the true eigenvalue: For adaptive STS integrators, the error is approximately independent of the used estimate, whereas for fixed integrators it can modify the used timestep. A tigher estimate for a fixed integrator will increase the timestep and hence the error. But let us assume (as given by the data) that spatial error dominates over temporal error, then for approximately the same error we only need to look at RHS evaluations to figure out how it influences the speedup.

For the STS integrators the number of RHS evaluations scales as $S = \sqrt{\frac{\Delta t_g}{\Delta t_e}}$ with the goal time step Δt_g to achieve some error and the stable Euler step $\Delta t_e = \frac{2}{\lambda}$; for the remaining integrators it is a simple proportionality. Hence being off by a factor of two in the timestep slows down the STS integrators by a factor of $\sqrt{2}$ and the rest by a factor of 2. Since the estimates were generally within a factor of two of the time step at which the FEuler integrator produced numerical instability, the RHS based speedups are at worst off by a factor of $\sqrt{\frac{1}{2}}$. Note though that the STS schemes use $0.9\Delta t_e$ for their stage estimate and hence may be said to actually be $\sqrt{\frac{1}{0.9}}$ times faster if actually ran at the stability limit.

Estimating the eigenvalues without the equality of the Gibbs energy prefactors produces extremely long expressions which are likely to be overestimates again. In general, a method for calculating the eigenvalue of the nonlinear RHS operator should be more efficient, especially if it doesn't need frequent recalculation. In that case one may e.g. calculate the PDE on accelerators and calculate regular updates for the maximum eigenvalue on CPU cores, using a snapshot of the PDE state. On step rejection the eigenvalue estimate may then be calculated directly from the current PDE data on the accelerator.