Meeting 22/10/2020

1 Mulitple Species Gradient Equation

We will need to consider the Frechét derivative of terms involving $F(\mathbf{w})$ first. From the definition from the Frechét derivative, we know that we have to consider the first order term of the Taylor expansion, so that we have:

$$F(\mathbf{w}+\mathbf{h}) - F(\mathbf{w}) = \nabla F(\mathbf{w}) \cdot \mathbf{h}.$$

However, this doesn't seem quite right. Consider from year end review: $F(\rho) = \nabla \ln(\rho)$. The resulting Frechét derivative was $\nabla(\frac{h}{\rho})$, which doesn't match with the above definition.
The form $F(\mathbf{w}) = w_1^2 + w_2^3$ that we suggested I tried to check this works does match the above definition.

2 Problem with InterpolationPhys Matrix

When we have a multishape of more than one shape the interpolation matrix seems to be wrong. However, I cannot figure out why. I have run three examples: one with a rectangle and a wedge, where it is clearly the wedge that is wrong (see Figure 1) and two examples with two rectangle, where again the second rectangle is wrong, see Figures 2, 3. This is interpolating from $N = 20$ to $N = 40$ but from 10 to 20 looks the same. I am not sure whether the problem is in my setup or in the implementation of the interpolation matrix (no screenshots of that here – will share my screen). If I change the order of the two shapes in Example 3, I get something even worse, see Figure 4.

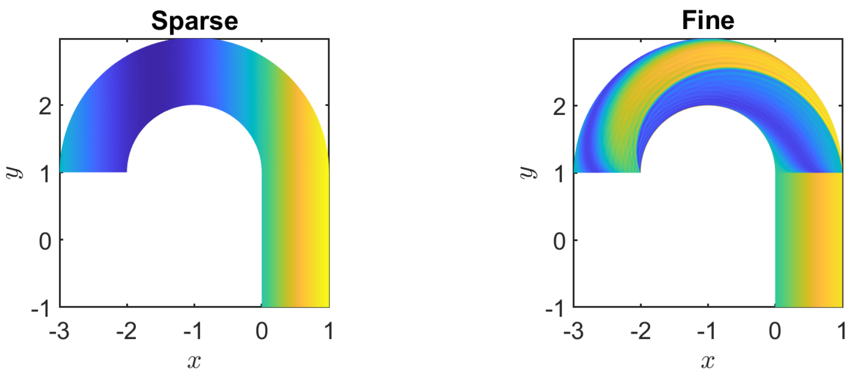

Figure 1: Example 1

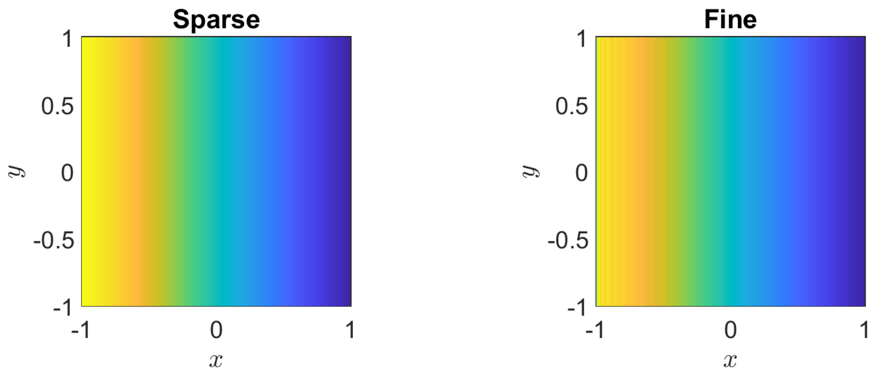

Figure 2: Example 2

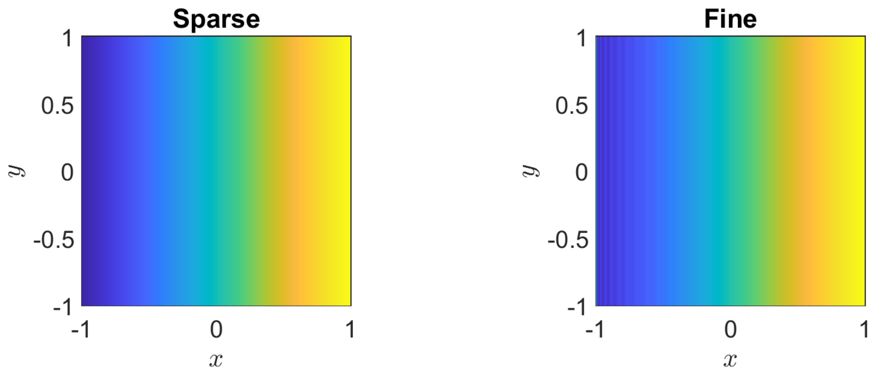

Figure 3: Example 3

3 Sedimentation Paper

We have:

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left(\Gamma \rho \nabla \frac{\delta F[\rho]}{\delta \rho} \right)$$
$$F[\rho] = k_B T \int \rho(\ln(\rho) - 1) dr + \int \rho V_{ext} dr + F_{exc}[\rho],$$

with:

$$V_{ext} = \frac{k_B T z}{\xi}, \quad \xi = \frac{k_B T}{mg} \qquad \text{for} \quad \sigma/2 < z < L - \sigma/2.$$

What's σ, the particle diameter, in our case?

Then we have Γ, which is defined as:

$$\Gamma_{HI}/\Gamma_0 = (1 - \phi^3)/[1 + 2\phi + 1.492\phi(1 - \phi^3)],$$
$$\phi = 4\pi\rho a^3/3,$$

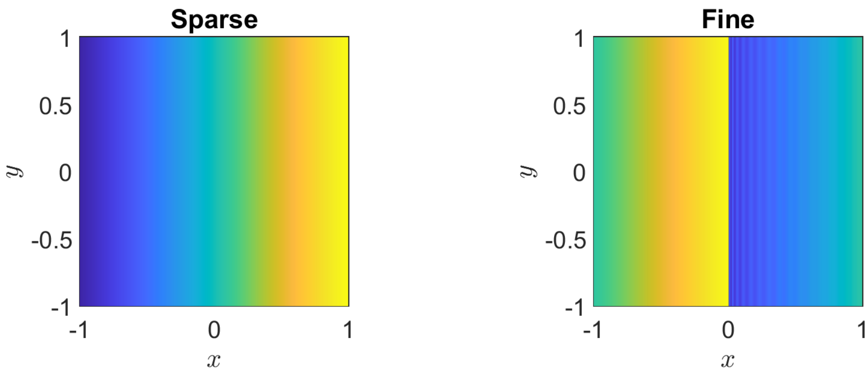

Figure 4: Example 4

where a is the particle radius. However, in the simulations we use the constant mobility, with overall packing fraction ϕ_0:

$$\Gamma_{HI}(\phi_0), \quad \phi_0 = \pi\sigma^3\nu/6L.$$

What is ν (the number density per area)? and do we have to scale the above formula by $\Gamma_0 = (6\pi\mu a)^{-1}$ (which I am not sure is the right expression)? Overall, I think we could just implement the values they chose in their table. But their F_{exc} will be different from ours, so I don't know whether that makes sense. The paper uses Rosenfeld's FMT.

4 Constriction Paper

We have:

$$\frac{\partial\rho}{\partial t} = \nabla\cdot\left(\rho\nabla\frac{\delta F[\rho]}{\delta\rho}\right)$$
$$F[\rho] = k_BT\int\rho(\ln(\rho)-1)dr + \int\rho(V_{ext}-fx)dr + F_{exc}[\rho],$$

where $f = k_BT/l$, l is a unit length (interparticle distance). Further:

$$V_{ext} = V_0[1 - 0.5erf((y+g(x))/\sqrt{2}w) + 0.5erf((y-g(x))/\sqrt{2}w)]$$

$$\begin{aligned} g(x) &= L_y/2 - \alpha[1+\cos(2\pi(x-x_0)/L_c)] \quad \text{for} \quad |x-x_0| < L_c/2, \\ &= L_y/2 \quad \text{otherwise} \\ \alpha &= (L_y/4)(1-b), \end{aligned}$$

where L_y is the channel height and L_c is the constriction width, b is the parameter that decides constriction height.

Q: What is w? How do we find l? How do we know the number of particles in DDFT? Formula $\rho_0 = N/A_0 = 1/l^2$.
Then we have $\Gamma = u_0 \rho_0^{3/2}/(k_B T)$, which is the measurement of interaction strength they use, so I need to know ρ_0.
Question: The form of $F_{exc}[\rho]$ involves $c_0^{(2)}$, the pair direct correlation function, which is different from our implementation.
Do we model in a box that's bigger or equal to L_y.