# Speed Up Analysis for Hybrid Grains

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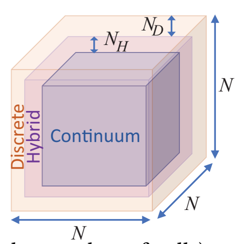
## 1 SUGAR COATED HYBRIDIZATION

Suppose that we have a chunk of granular material in a cubic shape (inset) with the total number of grains $A$. We are interested in using our hybrid grains approach to simulate such material, where we first set a grid covering the cubic region with the resolution (number of cells) $N > 0$ in each dimension, then set the outmost $N_D > 0$ layers (in terms of the number of cells) as purely discrete, their inner $N_H > 0$ layers as hybrid, and the innermost $N-2N_D-2N_H$ layers as purely continuum. We now derive the optimal setting of $N$, $N_D$ and $N_H$ that gives us the maximum speed up over a purely discrete simulation for the entire cubic shaped chunk of granular material.




### 1.1 A Model for the Computation Cost

We first describe our model for the per-step computation cost of the purely discrete and our hybrid simulations. Let $C_D$ be the (per-step) cost for processing each grain in the discrete simulation. Then the per-step cost of the purely discrete simulation $T_C$ is $C_D$ multiplied by the total number of grains $A$:

$$T_C = C_D A.$$

The total cost of the hybrid simulation $T_H$ is the sum of the costs of the enrichment, discrete and continuum steps. Let $C_E$ be the (per-step) cost for processing each cell in the enrichment. The total cost of enrichment per step can then be written as $C_E N^3$. It scales with $N^3$ because we compute the level set function for each cell. In a hybrid simulation, we only have grains in the purely discrete and hybrid regions. The number of cells containing grains can be computed by subtracting the number of purely continuum cells $(N - 2N_H - 2N_D)^3$ from the total number of cells $N^3$, so the total number of grains can be written as $A\{N^3 - (N - 2N_H - 2N_D)^3\}/N^3$, which gives us the per-step discrete cost as $C_D A\{N^3 - (N - 2N_H - 2N_D)^3\}/N^3$. Likewise, the per-step continuum cost can be described as $C_C(N - 2N_D)^3$, where $C_C$ is the (per-step) cost for processing each cell in the continuum simulation. In summary, we have

$$T_H = C_E N^3 + C_D A \frac{N^3 - (N - 2N_H - 2N_D)^3}{N^3} + C_C(N - 2N_D)^3.$$

In our hybrid simulation, the frequencies of performing enrichment and mpm integration are lower than that of the discrete integration. Hence as for $C_E$ and $C_C$, we are considering the amortized cost (i.e., the true cost during the performance step divided by the interval).

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### 1.2 The Reduction Ratio in the Computation Time

Next, for a fixed number of total effective grains $A$ (we refer to the number of 'effective' grains as the number of total grains in the purely discrete counterpart), we define the reduction ratio $R_A$ in the computation time between $T_H$ and $T_C$ as

$$\begin{aligned} R_A(N, N_D, N_H) &= \frac{T_H}{T_C} \\ &= \frac{C_E}{C_D A} N^3 + \frac{N^3 - (N - 2N_H - 2N_D)^3}{N^3} + \frac{C_C}{C_D A}(N - 2N_D)^3. \end{aligned} \quad (1)$$

With this model, we seek for the parameters $N$, $N_D$, and $N_H$ that minimize $R_A$ for a maximized speed-up.

### 1.3 Determining $N_H$

To analyze how $R_A$ changes with respect to $N_H$, we compute the partial derivative of $R_A$ with respect to $N_H$ as

$$\frac{\partial R_A(N, N_D, N_H)}{\partial N_H} = \frac{6}{N^3}(N - 2N_H - 2N_D)^2 \geq 0,$$

and find that $\frac{\partial R_A}{\partial N_H}$ is non negative, meaning that $R_A$ is a non decreasing function with respect to $N_H$. Hence to minimize $R_A$, we take the smallest possible value for $N_H$. Because $N_H$ only takes positive integer values, we arrive at $N_H = 1$.

## 1.4 Determining $N_D$

Next, we substitute $N_H = 1$ into (1) and compute the partial derivative of $R_A$ with respect to $N_D$ to find the optimal $N_D$:

$$\begin{aligned}\frac{\partial R_A(N, N_D, N_H = 1)}{\partial N_D} &= \frac{6}{N^3}(N-2-2N_D)^2 - 6\frac{C_C}{C_D A}(N-2N_D)^2 \\ = N_D^2 \underbrace{\left(\frac{24}{N^3} - \frac{24 C_C}{C_D A}\right)}_{\alpha} &+ N_D \underbrace{\left(-24\frac{N-2}{N^3} + 24\frac{N C_C}{C_D A}\right)}_{\beta} \\ &+ \underbrace{\frac{6(N-2)^2}{N^3} - \frac{6 C_C N^2}{C_D A}}_{\gamma}. \end{aligned} \tag{2}$$

(2) is a quadratic function. We let $\alpha$, $\beta$, and $\gamma$ be the coefficients, and investigate their characteristics. We introduce $R_D$ to denote the number of grains per cell, with which $A$ and $N$ are related via $A = R_D N^3$. With this convention, $\alpha = \frac{24}{N^3}\left(1 - \frac{C_C}{C_D R_D}\right)$. Note that $C_D R_D$ and $C_C$ are respectively the per-cell costs of discrete and continuum simulations. In hybrid grains, we are interested in making use of continuum homogenization to accelerate the corresponding discrete simulation, therefore $C_C < C_D R_D$ is the typical use case of hybrid grains. Thus, $\alpha > 0$. Likewise, with $A = R_D N^3$, we have $\beta = -\frac{24}{N^2}\left(\left(1 - \frac{2}{N}\right) - \frac{C_C}{C_D R_D}\right)$. As $N$ increases, $1 - \frac{2}{N}$ approaches 1, and following the discussion of $\alpha$, $\left(1 - \frac{2}{N}\right) > \frac{C_C}{C_D R_D}$ is our typical use case, so $\beta < 0$. Finally, $\gamma = \frac{6}{N}\left(\left(1 - \frac{2}{N}\right)^2 - \frac{C_C}{C_D R_D}\right)$, and again, we typically have $\left(1 - \frac{2}{N}\right)^2 > \frac{C_C}{C_D R_D}$, so $\gamma > 0$.

With $\alpha > 0$, $\beta < 0$, and $\gamma > 0$, we know that the quadratic function $\frac{\partial R_A}{\partial N_D}$ is convex downward, and that the two solutions $\eta_1$ and $\eta_2$ (with $\eta_1 < \eta_2$) of $\frac{\partial R_A}{\partial N_D} = 0$ are both positive. Thus, the function of $R_A$ with respect to $N_D$ increases while $N_D < \eta_1$, then, it has a local maximum at $N_D = \eta_1$, starts to decrease while $\eta_1 < N_D < \eta_2$, has a local minimum at $\eta_2$ and then increases for $N_D > \eta_2$. Thus, in the region $N_D > 0$, the global minimum is either at $N_D = 1$ or $N_D = \eta_2$. Now we see that $N_D = \eta_2$ is not appropriate. First, we compute

$$\begin{aligned}\eta_2 &= \frac{-\beta/2 + \sqrt{(\beta/2)^2 - \alpha\gamma}}{\alpha} = \frac{N(1 - \frac{C_C}{C_D R_D}) + 2(\sqrt{\frac{C_C}{C_D R_D}} - 1)}{2(1 - \frac{C_C}{C_D R_D})} \\ &= \frac{N}{2} - \frac{1}{\sqrt{\frac{C_C}{C_D R_D}} + 1} > \frac{N-2}{2}.\end{aligned}$$

With $N_D = \eta_2$, we have a violation $2(N_D + N_H) > N$, and hence inappropriate. Thus we arrive at $N_D = 1$.

## 1.5 Determining $N$

With $N_H = 1$ and $N_D = 1$, $R_A$ becomes

$$R_A(N) = \frac{C_E}{C_D A}N^3 + \frac{12N^2 - 48N + 64}{N^3} + \frac{C_C}{C_D A}(N-2)^3.$$

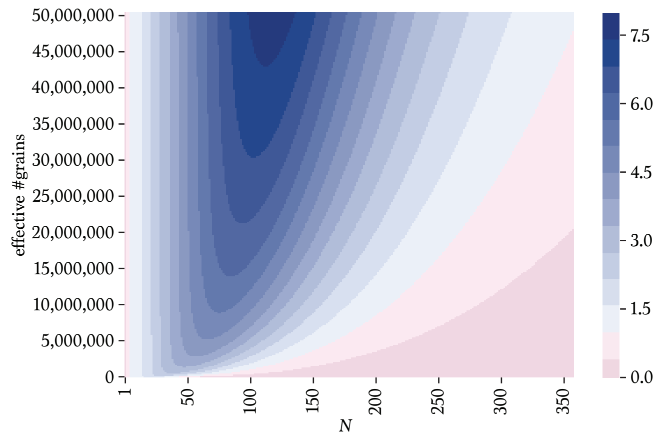



Fig. 1. We show how the acceleration ratio of our hybrid grains ($1/R_A(N)$) according to $N$ (horizontal axis) and $A$ (vertical axis). Reddish color indicates the case where the hybrid grains is slower than the purely discrete, and darker blue indicates more speed up with hybrid grains.

Figure 1 shows a plot of the acceleration ratio $1.0/R_A(N)$ for various $N$ and $A$. To find the optimal $N$, we compute

$$\begin{aligned}\frac{\partial R_A(N)}{\partial N} &= \frac{3C_E}{C_D A}N^2 - \frac{12}{N^2} + \frac{96}{N^3} - \frac{192}{N^4} + \frac{3C_C}{C_D A}(N-2)^2 \\ &= \frac{3}{N^4}\left(\frac{C_E}{C_D A}N^6 + \frac{C_C}{C_D A}N^4(N-2)^2 - 4(N-4)^2\right) \\ &= \frac{12}{N^4}\left(\underbrace{\frac{C_E + C_C}{4 C_D A}}_{\frac{1}{K}} N^4\left(N^2 + \underbrace{\frac{4C_C}{C_E + C_C}}_{B}(1-N)\right) - (N-4)^2\right) \\ &= \frac{12}{N^4}\left(\frac{N^4}{K}\left(N^2 + B(1-N)\right) - (N-4)^2\right),\end{aligned}$$

where we have set $\frac{1}{K} = \frac{C_E + C_C}{4 C_D A}$, and $B = \frac{4C_C}{C_E + C_C}$. Note that $K$ scales with $A$ linearly.

When $\frac{\partial R_A(N)}{\partial N} = 0$, any changes in the discrete computation time will be (marginally) balanced by the changes in the enrichment and continuum computation time.

Finding the local extrema of $R_A(N)$ amounts to solving

$$f(N) := \frac{N^4}{K}\left(N^2 + B(1-N)\right) - (N-4)^2 = 0. \tag{3}$$

$f(N) = 0$ has two types of solutions. One is in the form $N = 4 + \epsilon$, because when $A$ (and consequently $K$) is large, the first term vanishes and the second term becomes dominant. However, this type of solutions is not our interest, because $N = 4 + \epsilon$ is almost purely discrete. The other type of solutions is $N = \pm K^{1/4}(1 + \epsilon)$, because then $\frac{N^4}{K} \approx 1$ and the remaining terms are both second order with opposite signs, so they cancel out. We are interested in positive $N$, so $N = K^{1/4}(1 + \epsilon)$.

Now, we will see that $N = K^{1/4}$ is truly the asymptotic solution to $f(N) = 0$. By assumption, $\epsilon \ll 1$, and we will see that $\epsilon \to 0$ as $K \to \infty$. Substituting $N = K^{1/4}(1 + \epsilon)$ into (3) and dropping higher orders of $\epsilon$, we have

$$f(N = K^{1/4}(1+\epsilon)) \approx \epsilon\left(4K^{1/2} + (8-5B)K^{1/4} + 4B\right) + \left((8-B)K^{1/4} + B - 16\right). \quad (4)$$

Solving (4) for $f = 0$ gives us

$$\epsilon = \frac{16 - B - (8-B)K^{1/4}}{4K^{1/2} + (8-5B)K^{1/4} + 4B} = \frac{\frac{16-B}{K^{1/2}} - \frac{(8-B)}{K^{1/4}}}{4 + \frac{(8-5B)}{K^{1/4}} + \frac{4B}{K^{1/2}}},$$

which goes to 0 as $K \to \infty$, hence

$$N = K^{1/4} = \left(\frac{4C_D A}{C_E + C_C}\right)^{1/4} \quad (5)$$

is the asymptotic solution. Since $f(N) \to \infty$ as $N \to \infty$, the largest solution (i.e., $N = K^{1/4}$) for $f(N) = 0$ corresponds to a local minimum of $R_A(N)$, which is what we are interested in.

### 1.6 Asymptotic Behavior of $R_A$ for Larger $A$

With (5), $R_A(N)$ becomes

$$R_A = \frac{4C_E}{C_E + C_C}\frac{1}{K^{1/4}} + \frac{12}{K^{1/4}} - \frac{48}{K^{2/4}} + \frac{64}{K^{3/4}} + \frac{4C_C}{C_E + C_C}\frac{(1 - \frac{2}{K^{1/4}})^3}{K^{1/4}}.$$

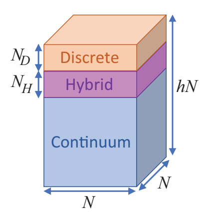
Therefore, as $A \to \infty$, $K \to \infty$, and then $R_A \to 0$, meaning that the speed up with our hybrid approach is *unbounded* and becomes arbitrarily large as we increase the total number of effective grains $A$ (as in Figure 1). The key is to set the grid resolution $N$ according to (5), with $N_H = 1$ and $N_D = 1$.

### 1.7 Intuitive Explanation

It is important to note that $N$ scales with $A$ in the power of 1/4, not 1/3. An intuitive explanation is that if we refine both the discrete and continuum elements equally (this corresponds to setting $N \propto A^{1/3}$) while keeping the discrete layer thickness to be minimum, then the discrete computation time will scale in the order of $N^2$ whereas the continuum in $N^3$, so eventually the continuum computation time will be dominant, and we will hit a bound. However, if we refine them *differently* and maintain a balance between the two (i.e., setting $N \propto A^{1/4}$), then the acceleration continues.

## 2 LAYERED HYBRIDIZATION

Now, suppose that we have a chunk of granular material in a cuboid shape (inset) with equal width and depth, the height $h$ times larger than the width and depth, and the total number of grains $A$. In the *layered hybridization*, we first set a grid (with the same cubic cells as the sugar-coated hybridization) covering the cuboid region with the resolution (number of cells) $N$ in the horizontal dimensions and $hN$ in the vertical dimension. Then we set the top $N_D > 0$ layers (in terms of the number of cells) as purely discrete, their inner $N_H > 0$ layers as hybrid, and the bottom $N - N_D - N_H$ layers as purely continuum. We now derive the optimal setting of $N$, $N_D$ and $N_H$ that gives us the maximum speed up over a purely discrete simulation for the entire cuboid shaped chunk of granular material.




### 2.1 A Model for the Computation Cost

Same as the sugar-coated hybridization, let $C_D$, $C_E$, and $C_C$ be the amortized, per-step cost for processing each discrete grain, each cell in the enrichment and each cell in the continuum simulation, respectively. The per-step cost of the purely discrete simulation $T_C$ is $C_D A$, and that of the hybrid simulation $T_H$ is given by

$$T_H = C_E hN^3 + C_D A\frac{(N_D + N_H)N^2}{hN^3} + C_C(hN - N_D)N^2.$$

### 2.2 The Reduction Ratio in the Computation Time

The reduction ratio $R_A$ in the computation time between $T_H$ and $T_C$ for a fixed number of total effective grains $A$ is given by

$$R_A(N, N_D, N_H) = \frac{T_H}{T_C} = \frac{C_E}{C_D A}hN^3 + \frac{N_D + N_H}{hN} + \frac{C_C}{C_D A}(hN - N_D)N^2. \quad (6)$$

We seek for the parameters $N$, $N_D$, and $N_H$ that minimize $R_A$ for a maximized speed-up.

### 2.3 Determining $N_H$

The partial derivative of $R_A$ with respect to $N_H$ is given by

$$\frac{\partial R_A(N, N_D, N_H)}{\partial N_H} = \frac{1}{hN} \geq 0.$$

Again, this is non negative, and we find $N_H = 1$.

### 2.4 Determining $N_D$

Next, we substitute $N_H = 1$ into (6) and compute the partial derivative of $R_A$ with respect to $N_D$. Noting that $A = R_D hN^3$, where $R_D$ is the number of grains per cell, we have

$$\frac{\partial R_A(N, N_D, N_H = 1)}{\partial N_D} = \frac{1}{hN} - \frac{C_C}{C_D A}N^2 = \frac{1}{hN}\left(1 - \frac{C_C}{C_D R_D}\right) > 0.$$

Thus the optimal $N_D$ is $N_D = 1$.

### 2.5 Determining $N$

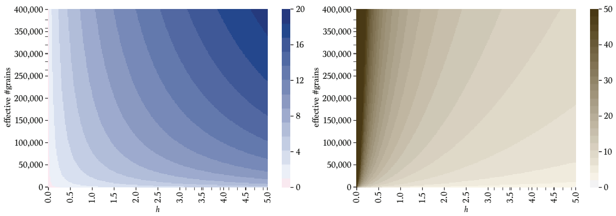
With $N_H = 1$ and $N_D = 1$, $R_A$ becomes

$$R_A(N) = \frac{C_E}{C_D A}hN^3 + \frac{2}{hN} + \frac{C_C}{C_D A}(hN - 1)N^2. \quad (7)$$

To find the optimal $N$, we compute

$$\begin{aligned}\frac{\partial R_A(N)}{\partial N} &= \frac{3hC_E}{C_D A}N^2 - \frac{2}{hN^2} + \frac{C_C}{C_D A}(3hN^2 - 2N) \\ &= \frac{2}{hN^3}\left(\frac{3h^2(C_E + C_C)}{2C_D A}N^5 - \frac{hC_C}{C_D A}N^4 - N\right) \\ &= \frac{2}{hN^3}\left(\underbrace{\frac{3h^2(C_E + C_C)}{2C_D A}}_{\frac{1}{K}}N^4\left(N - \underbrace{\frac{2C_C}{3h(C_E + C_C)}}_{B}\right) - N\right) \\ &= \frac{2}{hN^3}\left(\frac{N^4}{K}(N - B) - N\right),\end{aligned}$$

where we have set $\frac{1}{K} = \frac{3h^2(C_E + C_C)}{2C_D A}$, and $B = \frac{2C_C}{3h(C_E + C_C)}$. Note that $K$ scales with $A$ linearly.




(a) (b)

Fig. 2. (a) The acceleration ratio of layered hybridization ($1/R_A$) with respect to the aspect ratio $h$ (horizontal axis) and $A$ (vertical axis). Reddish color means the hybrid grains is slower than the purely discrete, and darker blue indicates more speed up with hybrid grains. (b) The optimal $N$ computed according to (10).

When $\frac{\partial R_A(N)}{\partial N} = 0$, any changes in the discrete computation time will be (marginally) balanced by the changes in the enrichment and continuum computation time.

Finding the local extrema of $R_A(N)$ amounts to solving

$$f(N) := \frac{N^4}{K}(N - B) - N = 0. \tag{8}$$

$f(N) = 0$ has two types of solutions. One is in the form $N = \epsilon$, because when $A$ (and consequently $K$) is large, the first term vanishes and the second term becomes dominant. However, this type of solutions is not our interest, because $N = \epsilon$ is almost purely discrete. The other type of solutions is $N = \pm K^{1/4}(1 + \epsilon)$, because then $\frac{N^4}{K} \approx 1$ and the remaining terms are both first order with opposite signs, so they cancel out. We are interested in positive $N$, so $N = K^{1/4}(1 + \epsilon)$.

Now, we will see that $N = K^{1/4}$ is truly the asymptotic solution to $f(N) = 0$. By assumption, $\epsilon \ll 1$, and we will see that $\epsilon \longrightarrow 0$ as $K \longrightarrow \infty$. Substituting $N = K^{1/4}(1 + \epsilon)$ into (8) and dropping higher orders of $\epsilon$, we have

$$\begin{aligned} f(N = K^{1/4}(1+\epsilon)) &= (1+\epsilon)^4(K^{1/4}(1+\epsilon) - B) - K^{1/4}(1+\epsilon) \\ &\approx (1 + 4\epsilon)(K^{1/4}\epsilon + K^{1/4} - B) - K^{1/4} - K^{1/4}\epsilon \\ &\approx \epsilon(4K^{1/4} - 4B) - B. \end{aligned} \tag{9}$$

Solving (9) for $f = 0$ gives us

$$\epsilon = \frac{B}{4K^{1/4} - 4B} = \frac{\frac{B}{4K^{1/4}}}{1 - \frac{B}{K^{1/4}}},$$

which goes to 0 as $K \longrightarrow \infty$, hence

$$N = K^{1/4} = \left(\frac{2C_D A}{3h^2(C_E + C_C)}\right)^{1/4} \tag{10}$$

is the asymptotic solution. Since $f(N) \longrightarrow \infty$ as $N \longrightarrow \infty$, the largest solution (i.e., $N = K^{1/4}$) for $f(N) = 0$ corresponds to a local minimum of $R_A(N)$, which is what we are interested in.

## 2.6 Asymptotic Behavior of $R_A$ for Larger $A$

With (10), $R_A(N)$ becomes

$$R_A = \frac{2C_E}{3h(C_E + C_C)K^{1/4}} + \frac{2}{hK^{1/4}} + \frac{2C_C}{3h^2(C_E + C_C)K^{1/4}}\left(h - \frac{1}{K^{1/4}}\right)$$

Therefore, as $A \longrightarrow \infty$, $K \longrightarrow \infty$, and then $R_A \longrightarrow 0$, meaning that the speed up of the layered hybridization with cubic cells is also *unbounded* and becomes arbitrarily large as we increase the total number of effective grains $A$ (as in Figure 2). The key is to set the grid resolution $N$ according to (10), with $N_H = 1$ and $N_D = 1$.

# 3 LAYERED HYBRIDIZATION IN 2D

Now, suppose that we have a chunk of granular material in a rectangular shape with the height $h$ times larger than the width, and the total number of grains $A$. We first set a grid (with cubic cells) covering the granular region with the number of cells $N$ in the horizontal dimension and $hN$ in the vertical dimension. Then we set the top $N_D > 0$ layers (in terms of the number of cells) as purely discrete, their inner $N_H > 0$ layers as hybrid, and the bottom $N - N_D - N_H$ layers as purely continuum. We now derive the optimal setting of $N$, $N_D$ and $N_H$ that gives us the maximum speed up over a purely discrete simulation for the entire rectangular shaped chunk of granular material.

## 3.1 A Model for the Computation Cost

Same as the sugar-coated hybridization, let $C_D$, $C_E$, and $C_C$ be the amortized, per-step cost for processing each discrete grain, each cell in the enrichment and each cell in the continuum simulation, respectively. The per-step cost of the purely discrete simulation $T_C$ is $C_D A$, and that of the hybrid simulation $T_H$ is given by

$$T_H = C_E hN^2 + C_D A\frac{(N_D + N_H)N}{hN^2} + C_C(hN - N_D)N.$$

## 3.2 The Reduction Ratio in the Computation Time

The reduction ratio $R_A$ in the computation time between $T_H$ and $T_C$ for a fixed number of total effective grains $A$ is given by

$$\begin{aligned} R_A(N, N_D, N_H) &= \frac{T_H}{T_C} \\ &= \frac{C_E}{C_D A}hN^2 + \frac{N_D + N_H}{hN} + \frac{C_C}{C_D A}(hN - N_D)N. \end{aligned} \tag{11}$$

We seek for the parameters $N$, $N_D$, and $N_H$ that minimize $R_A$ for a maximized speed-up.

## 3.3 Determining $N_H$

The partial derivative of $R_A$ with respect to $N_H$ is given by

$$\frac{\partial R_A(N, N_D, N_H)}{\partial N_H} = \frac{1}{hN} \geq 0.$$

Again, this is non negative, and we find $N_H = 1$.

## 3.4 Determining $N_D$

Next, we substitute $N_H = 1$ into (11) and compute the partial derivative of $R_A$ with respect to $N_D$. Noting that $A = R_D hN^2$, where $R_D$ is the number of grains per cell, we have

$$\frac{\partial R_A(N, N_D, N_H = 1)}{\partial N_D} = \frac{1}{hN} - \frac{C_C}{C_D A}N = \frac{1}{hN}\left(1 - \frac{C_C}{C_D R_D}\right) > 0.$$

Thus the optimal $N_D$ is $N_D = 1$.

### 3.5 Determining $N$

With $N_H = 1$ and $N_D = 1$, $R_A$ becomes

$$R_A(N) = \frac{C_E}{C_D A} h N^2 + \frac{2}{hN} + \frac{C_C}{C_D A}(hN - 1)N. \tag{12}$$

To find the optimal $N$, we compute

$$\begin{aligned}
\frac{\partial R_A(N)}{\partial N} &= \frac{2hC_E}{C_D A} N - \frac{2}{hN^2} + \frac{C_C}{C_D A}(2hN - 1) \\
&= \frac{2}{hN^3}\left(\frac{h^2(C_E + C_C)}{C_D A} N^4 - \frac{hC_C}{2C_D A} N^3 - N\right) \\
&= \frac{2}{hN^3}\left(\underbrace{\frac{h^2(C_E + C_C)}{C_D A}}_{\frac{1}{K}} N^3 \left(N - \underbrace{\frac{C_C}{2h(C_E + C_C)}}_{B}\right) - N\right) \\
&= \frac{2}{hN^3}\left(\frac{N^3}{K}(N - B) - N\right),
\end{aligned}$$

where we have set $\frac{1}{K} = \frac{h^2(C_E+C_C)}{C_D A}$, and $B = \frac{C_C}{2h(C_E+C_C)}$. Note that $K$ scales with $A$ linearly.

When $\frac{\partial R_A(N)}{\partial N} = 0$, any changes in the discrete computation time will be (marginally) balanced by the changes in the enrichment and continuum computation time.

Finding the local extrema of $R_A(N)$ amounts to solving

$$f(N) := \frac{N^3}{K}(N - B) - N = 0. \tag{13}$$

$f(N) = 0$ has two types of solutions. One is in the form $N = \epsilon$, because when $A$ (and consequently $K$) is large, the first term vanishes and the second term becomes dominant. However, this type of solutions is not our interest, because $N = \epsilon$ is almost purely discrete. The other type of solutions is $N = \pm K^{1/3}(1 + \epsilon)$, because then $\frac{N^3}{K} \approx 1$ and the remaining terms are both first order with opposite signs, so they cancel out. We are interested in positive $N$, so $N = K^{1/3}(1 + \epsilon)$.

Now, we will see that $N = K^{1/3}$ is truly the asymptotic solution to $f(N) = 0$. By assumption, $\epsilon \ll 1$, and we will see that $\epsilon \to 0$ as $K \to \infty$. Substituting $N = K^{1/3}(1 + \epsilon)$ into (13) and dropping higher orders of $\epsilon$, we have

$$\begin{aligned}
&f(N = K^{1/3}(1 + \epsilon)) = (1 + \epsilon)^3 (K^{1/3}(1 + \epsilon) - B) - K^{1/3}(1 + \epsilon) \\
&\approx (1 + 3\epsilon)(K^{1/3}\epsilon + K^{1/3} - B) - K^{1/3} - K^{1/3}\epsilon \\
&\approx \epsilon(3K^{1/3} - 3B) - B. 
\end{aligned} \tag{14}$$

Solving (14) for $f = 0$ gives us

$$\epsilon = \frac{B}{3K^{1/3} - 3B} = \frac{\frac{B}{3K^{1/3}}}{1 - \frac{B}{K^{1/3}}},$$

which goes to 0 as $K \to \infty$, hence

$$N = K^{1/3} = \left(\frac{C_D A}{h^2(C_E + C_C)}\right)^{1/3} \tag{15}$$

is the asymptotic solution. Since $f(N) \to \infty$ as $N \to \infty$, the largest solution (i.e., $N = K^{1/3}$) for $f(N) = 0$ corresponds to a local minimum of $R_A(N)$, which is what we are interested in.

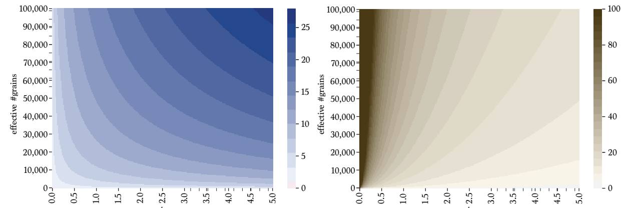



Fig. 3. (a) The acceleration ratio of layered hybridization ($1/R_A$) with respect to the aspect ratio $h$ (horizontal axis) and $A$ (vertical axis). Reddish color means the hybrid grains is slower than the purely discrete, and darker blue indicates more speed up with hybrid grains. (b) The optimal $N$ computed according to (15).

### 3.6 Asymptotic Behavior of $R_A$ for Larger $A$

With (15), $R_A(N)$ becomes

$$R_A = \frac{C_E}{h(C_E + C_C)K^{1/3}} + \frac{2}{hK^{1/3}} + \frac{C_C}{h^2(C_E + C_C)K^{1/3}}\left(h - \frac{1}{K^{1/3}}\right)$$

Therefore, as $A \to \infty$, $K \to \infty$, and then $R_A \to 0$, meaning that the speed up of the layered hybridization with cubic cells is also *unbounded* and becomes arbitrarily large as we increase the total number of effective grains $A$ (as in Figure 3). The key is to set the grid resolution $N$ according to (15), with $N_H = 1$ and $N_D = 1$.