CSE 548: Analysis of Algorithms

Lecture 4 (Divide-and-Conquer Algorithms: Polynomial Multiplication)

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$$A(x) = \sum_{j=0}^{n-1} a_j x^j$$

= $a_0 + a_1 x + a_2 x^2 + \dots + a_{n-1} x^{n-1}$

A(x) is a polynomial of degree bound n represented as a vector $a=(a_0,a_1,\cdots,a_{n-1})$ of coefficients.

The *degree* of A(x) is k provided it is the largest integer such that a_k is nonzero. Clearly, $0 \le k \le n-1$.

Evaluating A(x) at a given point:

Takes $\Theta(n)$ time using Horner's rule:

$$A(x_0) = a_0 + a_1 x_0 + a_2 (x_0)^2 + \dots + a_{n-1} (x_0)^{n-1}$$

= $a_0 + x_0 \left(a_1 + x_0 \left(a_2 + \dots + x_0 \left(a_{n-2} + x_0 (a_{n-1}) \right) \dots \right) \right)$

Adding Two Polynomials:

Adding two polynomials of degree bound n takes $\Theta(n)$ time.

$$C(x) = A(x) + B(x)$$

where,
$$A(x) = \sum_{j=0}^{n-1} a_j x^j$$
 and $B(x) = \sum_{j=0}^{n-1} b_j x^j$.

Then
$$C(x) = \sum_{j=0}^{n-1} c_j x^j$$
, where, $c_j = a_j + b_j$ for $0 \le j \le n-1$.

Multiplying Two Polynomials:

The product of two polynomials of degree bound n is another polynomial of degree bound 2n-1.

$$C(x) = A(x)B(x)$$

where,
$$A(x) = \sum_{j=0}^{n-1} a_j x^j$$
 and $B(x) = \sum_{j=0}^{n-1} b_j x^j$.

Then
$$C(x) = \sum_{j=0}^{2n-2} c_j x_j^j$$
 where, $c_j = \sum_{k=0}^{j} a_k b_{j-k}$ for $0 \le j \le 2n-2$.

The coefficient vector $c=(c_0,c_1,\cdots,c_{2n-2})$, denoted by $c=a\otimes b$, is also called the *convolution* of vectors $a=(a_0,a_1,\cdots,a_{n-1})$ and $b=(b_0,b_1,\cdots,b_{n-1})$.

Clearly, straightforward evaluation of c takes $\Theta(n^2)$ time.

$$\begin{bmatrix} a_0 \\ b_3x^3 \\ \end{bmatrix} + \begin{bmatrix} a_0x^2 \\ b_2x^2 \\ \end{bmatrix} + \begin{bmatrix} a_1x \\ b_1x \\ \end{bmatrix} + \begin{bmatrix} b_0 \\ a_0b_2x^2 \\ \end{bmatrix} + \begin{bmatrix} a_1b_1x^2 \\ \end{bmatrix} + \begin{bmatrix} a_2b_0x^2 \\ \end{bmatrix}$$

$$\begin{vmatrix} a_0 & + & a_1x & + & a_2x^2 & + & a_3x^3 \\ b_3x^3 & + & b_2x^2 & + & b_1x & + & b_0 \\ a_0b_3x^3 & + & a_1b_2x^3 & + & a_2b_1x^3 & + & a_3b_0x^3 \end{vmatrix}$$

Multiplying Two Polynomials:

We can use Karatsuba's algorithm (assume n to be a power of 2):

$$A(x) = \sum_{j=0}^{n-1} a_j x^j = \sum_{j=0}^{\frac{n}{2}-1} a_j x^j + x^{\frac{n}{2}} \sum_{j=0}^{\frac{n}{2}-1} a_{\frac{n}{2}+j} x^j = A_1(x) + x^{\frac{n}{2}} A_2(x)$$

$$B(x) = \sum_{j=0}^{n-1} b_j x^j = \sum_{j=0}^{\frac{n}{2}-1} b_j x^j + x^{\frac{n}{2}} \sum_{j=0}^{\frac{n}{2}-1} b_{\frac{n}{2}+j} x^j = B_1(x) + x^{\frac{n}{2}} B_2(x)$$

Then
$$C(x) = A(x)B(x)$$

= $A_1(x)B_1(x) + x^{\frac{n}{2}}[A_1(x)B_2(x) + A_2(x)B_1(x)] + x^n A_2(x)B_2(x)$

But
$$A_1(x)B_2(x) + A_2(x)B_1(x)$$

= $[A_1(x) + A_2(x)][B_1(x) + B_2(x)] - A_1(x)B_1(x) - A_2(x)B_2(x)$

3 recursive multiplications of polynomials of degree bound $\frac{n}{2}$.

Similar recurrence as in Karatsuba's integer multiplication algorithm leading to a complexity of $O(n^{\log_2 3}) = O(n^{1.59})$.

Point-Value Representation of Polynomials

A point-value representation of a polynomial A(x) is a set of n point-value pairs $\{(x_0, y_0), (x_1, y_1), ..., (x_{n-1}, y_{n-1})\}$ such that all x_k are distinct and $y_k = A(x_k)$ for $0 \le k \le n-1$.

A polynomial has many point-value representations.

Adding Two Polynomials:

Suppose we have point-value representations of two polynomials of degree bound n using the same set of n points.

$$A: \{(x_0, y_0^a), (x_1, y_1^a), \dots, (x_{n-1}, y_{n-1}^a)\}$$

$$B: \{(x_0, y_0^b), (x_1, y_1^b), \dots, (x_{n-1}, y_{n-1}^b)\}$$

If
$$C(x) = A(x) + B(x)$$
 then
$$C: \{(x_0, y_0^a + y_0^b), (x_1, y_1^a + y_1^b), ..., (x_{n-1}, y_{n-1}^a + y_{n-1}^b)\}$$

Thus polynomial addition takes $\Theta(n)$ time.

Point-Value Representation of Polynomials

Multiplying Two Polynomials:

Suppose we have *extended* (why?) point-value representations of two polynomials of degree bound n using the same set of 2n points.

$$A: \{(x_0, y_0^a), (x_1, y_1^a), \dots, (x_{2n-1}, y_{2n-1}^a)\}$$

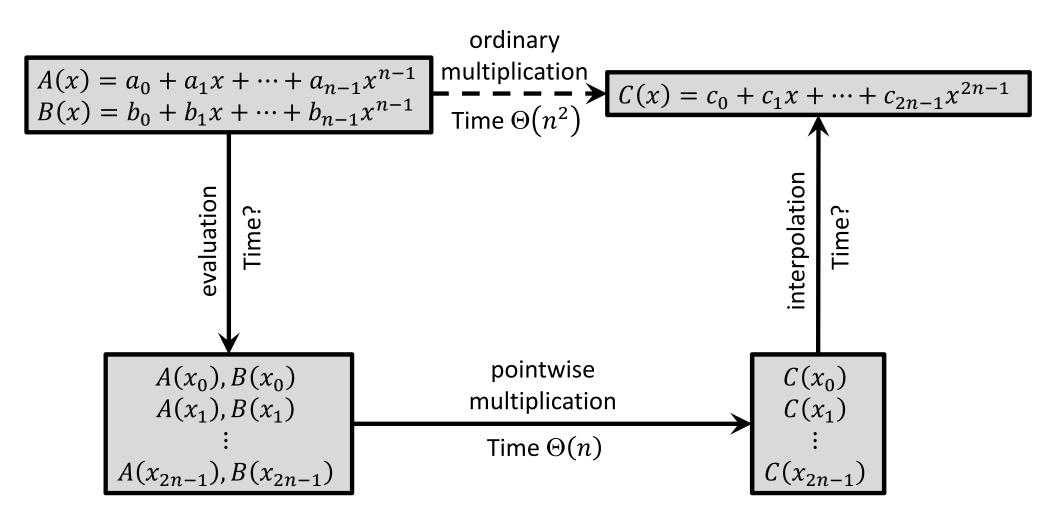
$$B: \{(x_0, y_0^b), (x_1, y_1^b), \dots, (x_{2n-1}, y_{2n-1}^b)\}$$

If C(x) = A(x)B(x) then

$$C: \{(x_0, y_0^a y_0^b), (x_1, y_1^a y_1^b), \dots, (x_{2n-1}, y_{2n-1}^a y_{2n-1}^b)\}$$

Thus polynomial multiplication also takes only $\Theta(n)$ time! (compare this with the $\Theta(n^2)$ time needed in the coefficient form)

<u>Faster Polynomial Multiplication?</u> (in Coefficient Form)



<u>Faster Polynomial Multiplication?</u> (in Coefficient Form)

Coefficient Representation ⇒ **Point-Value Representation**:

We select any set of n distinct points $\{x_0, x_1, ..., x_{n-1}\}$, and evaluate $A(x_k)$ for $0 \le k \le n-1$.

Using Horner's rule this approach takes $\Theta(n^2)$ time.

Point-Value Representation ⇒ **Coefficient Representation**:

We can interpolate using Lagrange's formula:

$$A(x) = \sum_{k=0}^{n-1} \frac{\prod_{j \neq k} (x - x_j)}{\prod_{j \neq k} (x_k - x_j)} y_k$$

This again takes $\Theta(n^2)$ time.

In both cases we need to do much better!

Coefficient Form \Rightarrow Point-Value Form

A polynomial of degree bound n: $A(x) = a_0 + a_1x + \cdots + a_{n-1}x^{n-1}$

A set of n distinct points: $\{x_0, x_1, ..., x_{n-1}\}$

Compute point-value form: $\{(x_0, A(x_0)), (x_1, A(x_1)), ..., (x_{n-1}, A(x_{n-1}))\}$

Using matrix notation:
$$\begin{bmatrix} A(x_0) \\ A(x_1) \\ \vdots \\ A(x_{n-1}) \end{bmatrix} = \begin{bmatrix} 1 & x_0 & (x_0)^2 & \cdots & (x_0)^{n-1} \\ 1 & x_1 & (x_1)^2 & \cdots & (x_1)^{n-1} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 1 & x_{n-1} & (x_{n-1})^2 & \cdots & (x_{n-1})^{n-1} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{bmatrix}$$

We want to choose the set of points in a way that simplifies the multiplication.

In the rest of the lecture on this topic we will assume:

n is a power of 2.

Let's choose $x_{n/2+j} = -x_j$ for $0 \le j \le n/2 - 1$. Then

$$\begin{bmatrix} A(x_0) \\ A(x_1) \\ \vdots \\ A(x_{n/2-1}) \\ A(x_{n/2+0}) \\ A(x_{n/2+1}) \\ \vdots \\ A(x_{n/2+(n/2-1)}) \end{bmatrix} = \begin{bmatrix} 1 & x_0 & (x_0)^2 & \cdots & (x_0)^{n-1} \\ 1 & x_1 & (x_1)^2 & \cdots & (x_1)^{n-1} \\ \vdots & \vdots & \ddots & \ddots & \cdots & \vdots \\ 1 & x_{n/2-1} & (x_{n/2-1})^2 & \cdots & (x_{n/2-1})^{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & -x_0 & (-x_0)^2 & \cdots & (-x_0)^{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & -x_{n/2-1} & (-x_{n/2-1})^2 & \cdots & (-x_{n/2-1})^{n-1} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ \vdots \\ a_{n-1} \end{bmatrix}$$

Observe that for
$$0 \le j \le n/2 - 1$$
: $(x_{n/2+j})^k = \begin{cases} (x_j)^k, & \text{if } k = even, \\ -(x_j)^k, & \text{if } k = odd. \end{cases}$

Thus we have just split the original $n \times n$ matrix into two almost similar $\frac{n}{2} \times n$ matrices!

How and how much do we save?

$$A(x) = \sum_{l=0}^{n-1} a_l x^l = \sum_{l=0}^{n/2-1} a_{2l} x^{2l} + \sum_{l=0}^{n/2-1} a_{2l+1} x^{2l+1}$$

$$= \sum_{l=0}^{n/2-1} a_{2l} (x^2)^l + x \sum_{l=0}^{n/2-1} a_{2l+1} (x^2)^l = A_{even}(x^2) + x A_{odd}(x^2),$$

where,
$$A_{even}(x) = \sum_{l=0}^{n/2-1} a_{2l}x^l$$
 and $A_{odd}(x) = \sum_{l=0}^{n/2-1} a_{2l+1}x^l$.

Observe that for
$$0 \le j \le n/2 - 1$$
: $A(x_j) = A_{even}(x_j^2) + x_j A_{odd}(x_j^2)$
 $A(x_{n/2+j}) = A(-x_j) = A_{even}(x_j^2) - x_j A_{odd}(x_j^2)$

So in order to evaluate $A(x_j)$ for all $0 \le j \le n-1$, we need:

n/2 evaluations of A_{even} and n/2 evaluations of A_{odd} n multiplications

n/2 additions and n/2 subtractions

Thus we save about half the computation!

If we can recursively evaluate A_{even} and A_{odd} using the same approach, we get the following recurrence relation for the running time of the algorithm:

$$T(n) = \begin{cases} \Theta(1), & if \ n = 1, \\ 2T(\frac{n}{2}) + \Theta(n), & otherwise. \end{cases}$$
$$= \Theta(n \log n)$$

Our trick was to evaluate A at x (positive) and -x (negative). But inputs to A_{even} and A_{odd} are always of the form x^2 (positive)! How can we apply the same trick?

Let us consider the evaluation of $A_{even}(x_j)$ for $0 \le j \le n/2 - 1$:

$$\begin{bmatrix} A_{even}(x_0) \\ A_{even}(x_1) \\ \vdots \\ A_{even}(x_{n/2-1}) \end{bmatrix} = \begin{bmatrix} 1 & (x_0)^2 & (x_0)^4 & \cdots & (x_0)^{n-2} \\ 1 & (x_1)^2 & (x_1)^4 & \cdots & (x_1)^{n-2} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 1 & (x_{n/2-1})^2 & (x_{n/2-1})^4 & \cdots & (x_{n/2-1})^{n-2} \end{bmatrix} \begin{bmatrix} a_0 \\ a_2 \\ a_4 \\ \vdots \\ a_{n-2} \end{bmatrix}$$

In order to apply the same trick on A_{even} we must set:

$$(x_{n/4+j})^2 = -(x_j)^2$$
 for $0 \le j \le n/4 - 1$

In A_{even} we set: $x_{n/4+j}^2 = -x_j^2$ for $0 \le j \le n/4 - 1$. Then

$$\begin{bmatrix} A_{even}(x_0) \\ A_{even}(x_1) \\ \vdots \\ A_{even}(x_{n/4-1}) \\ A_{even}(x_{n/4+0}) \\ A_{even}(x_{n/4+(n/4-1)}) \end{bmatrix} = \begin{bmatrix} 1 & x_0^2 & (x_0^2)^2 & \cdots & (x_0^2)^{\frac{n}{2}-1} \\ 1 & x_1^2 & (x_1^2)^2 & \cdots & (x_1^2)^{\frac{n}{2}-1} \\ \vdots & \vdots & \ddots & \cdots & \ddots & \vdots \\ 1 & x_{n/4-1}^2 & (x_{n/4-1}^2)^2 & \cdots & (x_{n/4-1}^2)^{\frac{n}{2}-1} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 1 & -x_0^2 & (-x_0^2)^2 & \cdots & (-x_0^2)^{\frac{n}{2}-1} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & -x_1^2 & (-x_1^2)^2 & \cdots & (-x_1^2)^{\frac{n}{2}-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & -x_{n/4-1}^2 & (-x_{n/2-1}^2)^2 & \cdots & (-x_{n/4-1}^2)^{\frac{n}{2}-1} \end{bmatrix} \begin{bmatrix} a_0 \\ a_2 \\ a_4 \\ \vdots \\ a_{n-2} \end{bmatrix}$$

This means setting $x_{n/4+j} = ix_j$, where $i = \sqrt{-1}$ (imaginary)!

This also allows us to apply the same trick on A_{odd} .

We can apply the trick once if we set:

$$x_{n/2+j} = -x_j \text{ for } 0 \le j \le n/2 - 1$$

We can apply the trick (recursively) 2 times if we also set:

$$(x_{n/2^2+j})^2 = -(x_j)^2$$
 for $0 \le j \le n/2^2 - 1$

We can apply the trick (recursively) 3 times if we also set:

$$\left(x_{n/2^3+j}\right)^{2^2} = -\left(x_j\right)^{2^2} \text{ for } 0 \le j \le n/2^3 - 1$$

We can apply the trick (recursively) k times if we also set:

$$(x_{n/2^k+j})^{2^{k-1}} = -(x_j)^{2^{k-1}}$$
 for $0 \le j \le n/2^k - 1$

Consider the t^{th} primitive root of unity:

$$\omega_t = e^{\frac{2\pi i}{t}} = \cos\frac{2\pi}{t} + i \cdot \sin\frac{2\pi}{t} \quad (i = \sqrt{-1})$$

Then

$$x_{n/2+j} = -x_j \implies x_{n/2^1+j} = \omega_{2^1} \cdot x_j$$

$$\left(x_{n/2^2+j}\right)^2 = -\left(x_j\right)^2 \implies x_{n/2^2+j} = \omega_{2^2} \cdot x_j$$

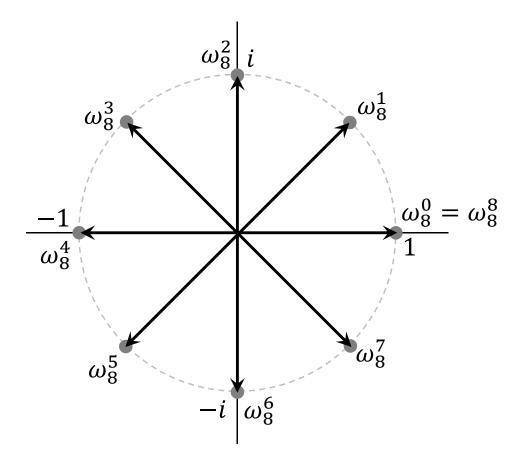
$$\left(x_{n/2^3+j}\right)^{2^2} = -\left(x_j\right)^{2^2} \implies x_{n/2^3+j} = \omega_{2^3} \cdot x_j$$

$$\left(x_{n/2^k+j}\right)^{2^{k-1}} = -\left(x_j\right)^{2^{k-1}} \implies x_{n/2^k+j} = \omega_{2^k} \cdot x_j$$

If $n=2^k$ we would like to apply the trick k times recursively. What values should we choose for $\{x_0, x_1, ..., x_{n-1}\}$?

Example: For $n = 2^3$ we need to choose $\{x_0, x_1, ..., x_7\}$.

Choose:
$$x_0 = 1$$
 $= \omega_8^0$
 $k = 3$: $x_1 = \omega_{2^3} \cdot x_0$ $= \omega_8^1$
 $k = 2$: $x_2 = \omega_{2^2} \cdot x_0$ $= \omega_8^2$
 $x_3 = \omega_{2^2} \cdot x_1$ $= \omega_8^3$
 $k = 1$: $x_4 = \omega_{2^1} \cdot x_0$ $= \omega_8^4$
 $x_5 = \omega_{2^1} \cdot x_1$ $= \omega_8^5$
 $x_6 = \omega_{2^1} \cdot x_2$ $= \omega_8^6$
 $x_7 = \omega_{2^1} \cdot x_3$ $= \omega_8^7$



complex 8^{th} roots of unity

For a polynomial of degree bound $n=2^k$, we need to apply the trick recursively at most $\log n=k$ times.

We choose $x_0 = 1 = \omega_n^0$ and set $x_j = \omega_n^j$ for $1 \le j \le n-1$.

Then we compute the following product:

$$\begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_{n-1} \end{bmatrix} = \begin{bmatrix} A(1) \\ A(\omega_n) \\ A(\omega_n^2) \\ \vdots \\ A(\omega_n^{n-1}) \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega_n & (\omega_n)^2 & \cdots & (\omega_n)^{n-1} \\ 1 & \omega_n^2 & (\omega_n^2)^2 & \cdots & (\omega_n^2)^{n-1} \\ \vdots & \vdots & \ddots & \ddots & \ddots \\ 1 & \omega_n^{n-1} & (\omega_n^{n-1})^2 & \cdots & (\omega_n^{n-1})^{n-1} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_{n-1} \end{bmatrix}$$

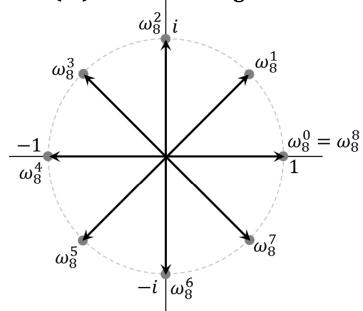
The vector $y=(y_0,y_1,\cdots,y_{n-1})$ is called the *discrete Fourier* transform (DFT) of (a_0,a_1,\cdots,a_{n-1}) .

This method of computing DFT is called the *fast Fourier transform* (FFT) method.

Example: For $n = 2^3 = 8$:

$$A(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 + a_6 x^6 + a_7 x^7$$

We need to evaluate A(x) at $x = \omega_8^i$ for $0 \le i < 8$.



complex 8^{th} roots of unity

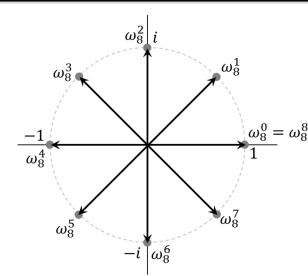
Now
$$A(x) = A_{even}(x^2) + x \cdot A_{odd}(x^2)$$
,

where
$$A_{even}(y) = a_0 + a_2 y + a_4 y^2 + a_6 y^3$$

and $A_{odd}(y) = a_1 + a_3 y + a_5 y^2 + a_7 y^3$

Observe that:

$$\omega_8^0 = \omega_8^8 = \omega_4^0$$
 $\omega_8^2 = \omega_8^{10} = \omega_4^1$
 $\omega_8^4 = \omega_8^{12} = \omega_4^2$
 $\omega_8^6 = \omega_8^{14} = \omega_4^3$



Also:

$$\omega_8^4 = -\omega_8^0$$

$$\omega_8^5 = -\omega_8^1$$

$$\omega_8^6 = -\omega_8^2$$

$$\omega_8^7 = -\omega_8^3$$

$$A(\omega_{8}^{0}) = A_{even}(\omega_{8}^{0}) + \omega_{8}^{0} \cdot A_{odd}(\omega_{8}^{0}) = A_{even}(\omega_{4}^{0}) + \omega_{8}^{0} \cdot A_{odd}(\omega_{4}^{0}),$$

$$A(\omega_{8}^{1}) = A_{even}(\omega_{8}^{2}) + \omega_{8}^{1} \cdot A_{odd}(\omega_{8}^{2}) = A_{even}(\omega_{4}^{1}) + \omega_{8}^{1} \cdot A_{odd}(\omega_{4}^{1}),$$

$$A(\omega_{8}^{2}) = A_{even}(\omega_{8}^{4}) + \omega_{8}^{2} \cdot A_{odd}(\omega_{8}^{4}) = A_{even}(\omega_{4}^{2}) + \omega_{8}^{2} \cdot A_{odd}(\omega_{4}^{2}),$$

$$A(\omega_{8}^{3}) = A_{even}(\omega_{8}^{6}) + \omega_{8}^{3} \cdot A_{odd}(\omega_{8}^{6}) = A_{even}(\omega_{4}^{3}) + \omega_{8}^{3} \cdot A_{odd}(\omega_{4}^{3}),$$

$$A(\omega_{8}^{4}) = A_{even}(\omega_{8}^{8}) + \omega_{8}^{4} \cdot A_{odd}(\omega_{8}^{8}) = A_{even}(\omega_{4}^{0}) - \omega_{8}^{0} \cdot A_{odd}(\omega_{4}^{0}),$$

$$A(\omega_{8}^{5}) = A_{even}(\omega_{8}^{10}) + \omega_{8}^{5} \cdot A_{odd}(\omega_{8}^{10}) = A_{even}(\omega_{4}^{1}) - \omega_{8}^{1} \cdot A_{odd}(\omega_{4}^{1}),$$

$$A(\omega_{8}^{6}) = A_{even}(\omega_{8}^{12}) + \omega_{8}^{6} \cdot A_{odd}(\omega_{8}^{12}) = A_{even}(\omega_{4}^{2}) - \omega_{8}^{2} \cdot A_{odd}(\omega_{4}^{2}),$$

$$A(\omega_{8}^{6}) = A_{even}(\omega_{8}^{12}) + \omega_{8}^{6} \cdot A_{odd}(\omega_{8}^{12}) = A_{even}(\omega_{4}^{2}) - \omega_{8}^{2} \cdot A_{odd}(\omega_{4}^{2}),$$

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$$A(\omega_{8}^{6}) = A_{even}(\omega_{8}^{12}) + \omega_{8}^{6} \cdot A_{odd}(\omega_{8}^{12}) = A_{even}(\omega_{4}^{2}) - \omega_{8}^{2} \cdot A_{odd}(\omega_{4}^{2}),$$

Rec-FFT ((
$$a_0$$
, a_1 , ..., a_{n-1}) { $n = 2^k$ for integer $k \ge 0$ }

1. if $n = 1$ then

2. return (a_0)

3. $\omega_n \leftarrow e^{2\pi i/n}$

4. $\omega \leftarrow 1$

5. $y^{\text{even}} \leftarrow \text{Rec-FFT}$ ((a_0 , a_2 , ..., a_{n-2}))

6. $y^{\text{odd}} \leftarrow \text{Rec-FFT}$ ((a_1 , a_3 , ..., a_{n-1}))

7. for $j \leftarrow 0$ to $n/2 - 1$ do

8. $y_j \leftarrow y_j^{\text{even}} + \omega y_j^{\text{odd}}$

9. $y_{n/2+j} \leftarrow y_j^{\text{even}} - \omega y_j^{\text{odd}}$

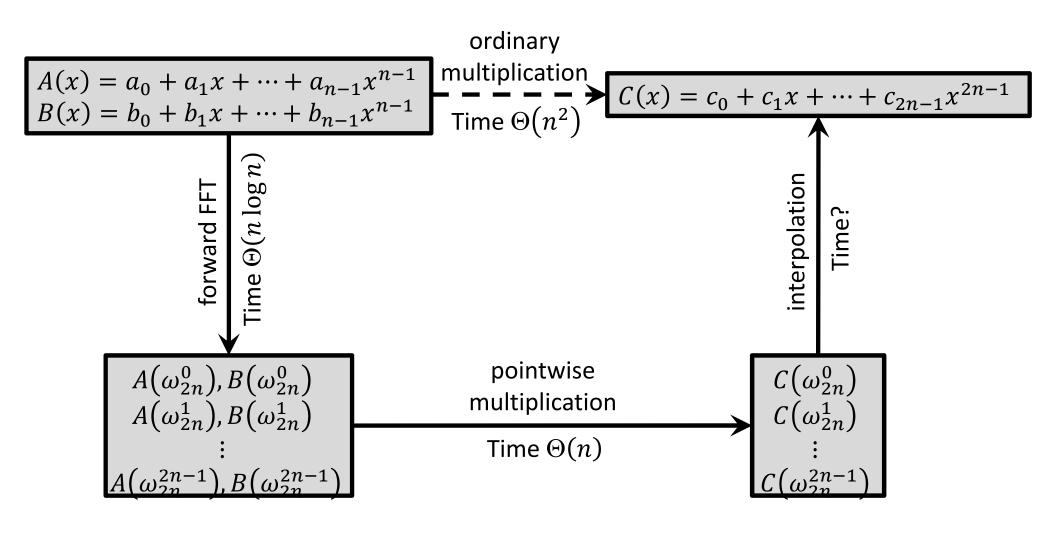
10. $\omega \leftarrow \omega \omega_n$

11. return y

Running time:

$$T(n) = \begin{cases} \Theta(1), & if \ n = 1, \\ 2T(\frac{n}{2}) + \Theta(n), & otherwise. \end{cases}$$
$$= \Theta(n \log n)$$

<u>Faster Polynomial Multiplication?</u> (in Coefficient Form)



Given:
$$\begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega_n & (\omega_n)^2 & \cdots & (\omega_n)^{n-1} \\ 1 & \omega_n^2 & (\omega_n^2)^2 & \cdots & (\omega_n^2)^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega_n^{n-1} & (\omega_n^{n-1})^2 & \cdots & (\omega_n^{n-1})^{n-1} \end{bmatrix} \underbrace{ \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_{n-1} \end{bmatrix}}_{V(\omega_n)} = \underbrace{ \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_{n-1} \end{bmatrix}}_{V(\omega_n)}$$

Vandermonde Matrix

$$\Rightarrow V(\omega_n) \cdot \bar{a} = \bar{y}$$

We want to solve: $\bar{a} = [V(\omega_n)]^{-1} \cdot \bar{y}$

It turns out that:
$$[V(\omega_n)]^{-1} = \frac{1}{n}V\left(\frac{1}{\omega_n}\right)$$

That means $[V(\omega_n)]^{-1}$ looks almost similar to $V(\omega_n)$!

Show that:
$$[V(\omega_n)]^{-1} = \frac{1}{n}V\left(\frac{1}{\omega_n}\right)$$

Let
$$U(\omega_n) = \frac{1}{n}V\left(\frac{1}{\omega_n}\right)$$

We want to show that $U(\omega_n)V(\omega_n)=I_n$, where I_n is the $n\times n$ identity matrix.

Observe that for $0 \le j, k \le n-1$, the $(j,k)^{th}$ entries are:

$$[V(\omega_n)]_{jk} = \omega_n^{jk}$$
 and $[U(\omega_n)]_{jk} = \frac{1}{n}\omega_n^{-jk}$

Then entry (p,q) of $U(\omega_n)V(\omega_n)$,

$$[U(\omega_n)V(\omega_n)]_{pq} = \sum_{k=0}^{n-1} [U(\omega_n)]_{pk} [V(\omega_n)]_{kq} = \frac{1}{n} \sum_{k=0}^{n-1} \omega_n^{k(q-p)}$$

$$[U(\omega_n)V(\omega_n)]_{pq} = \frac{1}{n} \sum_{k=0}^{n-1} \omega_n^{k(q-p)}$$

CASE p = q:

$$[U(\omega_n)V(\omega_n)]_{pq} = \frac{1}{n} \sum_{k=0}^{n-1} \omega_n^0 = \frac{1}{n} \sum_{k=0}^{n-1} 1 = \frac{1}{n} \times n = 1$$

CASE $p \neq q$:

$$[U(\omega_n)V(\omega_n)]_{pq} = \frac{1}{n} \sum_{k=0}^{n-1} (\omega_n^{q-p})^k = \frac{1}{n} \times \frac{(\omega_n^{q-p})^n - 1}{\omega_n^{q-p} - 1}$$
$$= \frac{1}{n} \times \frac{(\omega_n^n)^{q-p} - 1}{\omega_n^{q-p} - 1} = \frac{1}{n} \times \frac{(1)^{q-p} - 1}{\omega_n^{q-p} - 1} = 0$$

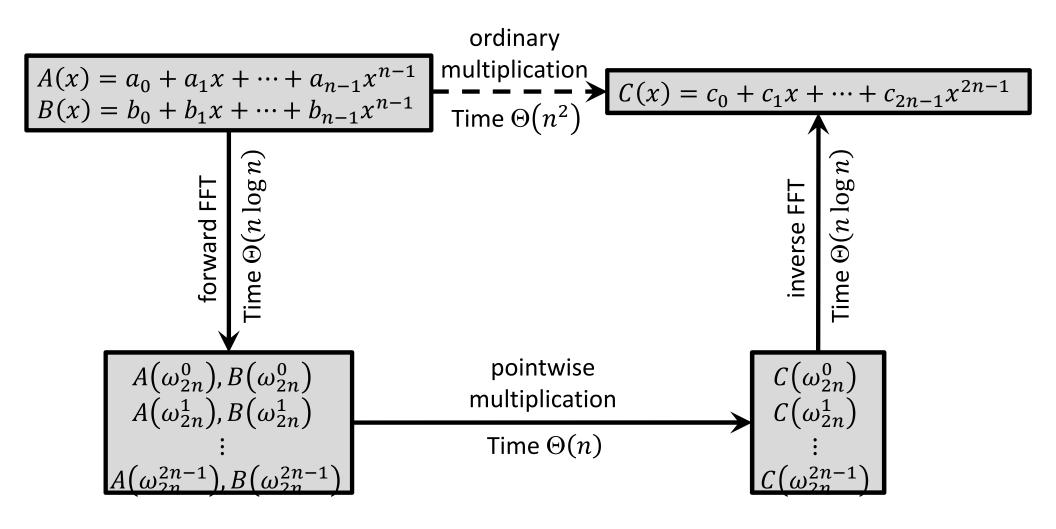
Hence $U(\omega_n)V(\omega_n) = I_n$

We need to compute the following matrix-vector product:

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_{n-1} \end{bmatrix} = \frac{1}{n} \times \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \frac{1}{\omega_n} & \left(\frac{1}{\omega_n}\right)^2 & \cdots & \left(\frac{1}{\omega_n}\right)^{n-1} \\ 1 & \frac{1}{\omega_n^2} & \left(\frac{1}{\omega_n^2}\right)^2 & \cdots & \left(\frac{1}{\omega_n^2}\right)^{n-1} \\ \vdots & \vdots & \ddots & \ddots & \ddots \\ \vdots & \vdots & \ddots & \ddots & \ddots \\ 1 & \frac{1}{\omega_n^{n-1}} & \left(\frac{1}{\omega_n^{n-1}}\right)^2 & \cdots & \left(\frac{1}{\omega_n^{n-1}}\right)^{n-1} \end{bmatrix} \underbrace{ \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_{n-1} \end{bmatrix} }_{\bar{y}}$$

This inverse problem is almost similar to the forward problem, and can be solved in $\Theta(n \log n)$ time using the same algorithm as the forward FFT with only minor modifications!

<u>Faster Polynomial Multiplication?</u> (in Coefficient Form)



Two polynomials of degree bound n given in the coefficient form can be multiplied in $\Theta(n \log n)$ time!

Some Applications of Fourier Transform and FFT

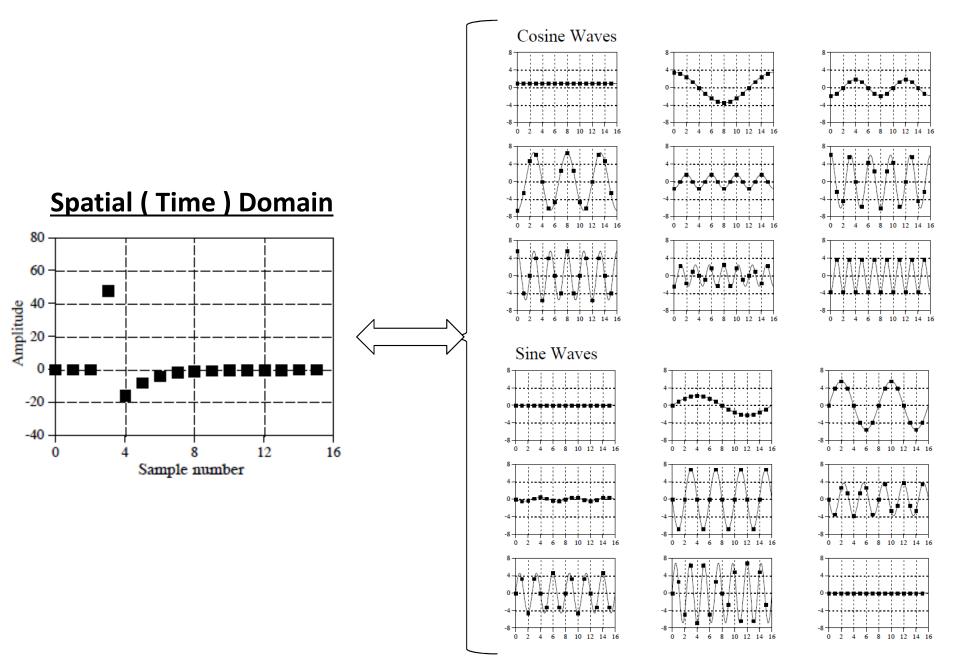
- Signal processing
- Image processing
- Noise reduction
- Data compression
- Solving partial differential equation
- Multiplication of large integers
- Polynomial multiplication
- Molecular docking

Some Applications of Fourier Transform and FFT

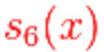


Any periodic signal can be represented as a sum of a series of sinusoidal (sine & cosine) waves. [1807]

Frequency Domain



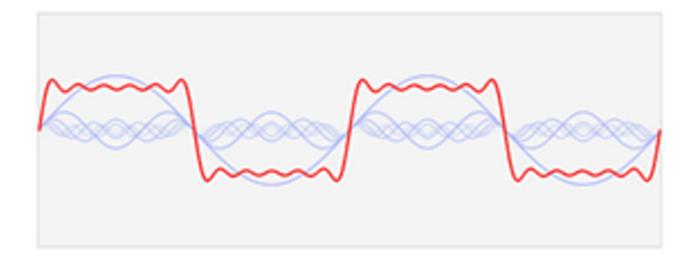
Source: The Scientist and Engineer's Guide to Digital Signal Processing by Steven W. Smith





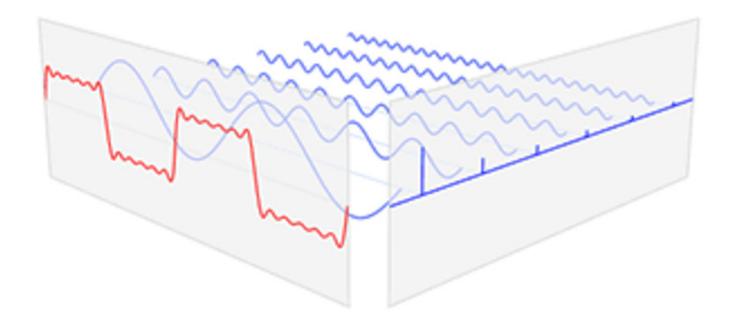
Function s(x) (in red) is a sum of six sine functions of different amplitudes and harmonically related frequencies. The Fourier transform, S(f) (in blue), which depicts amplitude vs frequency, reveals the 6 frequencies and their amplitudes.

$$s_6(x)$$



$$a_n \cos(nx) + b_n \sin(nx)$$

Function s(x) (in red) is a sum of six sine functions of different amplitudes and harmonically related frequencies. The Fourier transform, S(f) (in blue), which depicts amplitude vs frequency, reveals the 6 frequencies and their amplitudes.



Function s(x) (in red) is a sum of six sine functions of different amplitudes and harmonically related frequencies. The Fourier transform, S(f) (in blue), which depicts amplitude vs frequency, reveals the 6 frequencies and their amplitudes.



S(f)

Function s(x) (in red) is a sum of six sine functions of different amplitudes and harmonically related frequencies. The Fourier transform, S(f) (in blue), which depicts amplitude vs frequency, reveals the 6 frequencies and their amplitudes.



Function s(x) (in red) is a sum of six sine functions of different amplitudes and harmonically related frequencies. The Fourier transform, S(f) (in blue), which depicts amplitude vs frequency, reveals the 6 frequencies and their amplitudes.

<u>Spatial (Time) Domain ⇔ Frequency Domain</u> <u>(Fourier Transforms)</u>

Let s(t) be a signal specified in the time domain.

The strength of s(t) at frequency f is given by:

$$S(f) = \int_{-\infty}^{\infty} s(t) \cdot e^{-2\pi i f t} dt$$

Evaluating this integral for all values of f gives the frequency domain function.

Now s(t) can be retrieved by summing up the signal strengths at all possible frequencies:

$$s(t) = \int_{-\infty}^{\infty} S(f) \cdot e^{2\pi i f t} \, df$$

Why do the Transforms Work?

Let's try to get a little intuition behind why the transforms work. We will look at a very simple example.

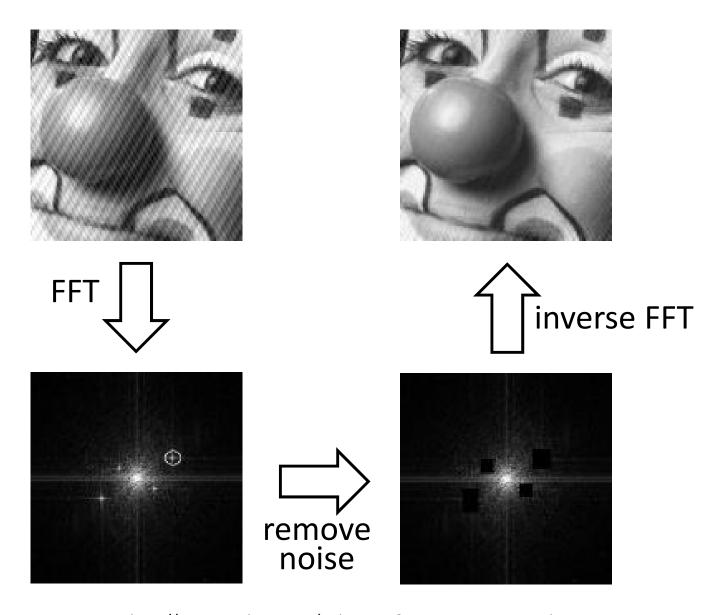
Suppose: $s(t) = \cos(2\pi h \cdot t)$

$$\frac{1}{T} \int_{-T}^{T} s(t) \cdot e^{-2\pi i f t} dt = \begin{cases} 1 + \frac{\sin(4\pi f T)}{4\pi f T}, & \text{if } f = h, \\ \frac{\sin(2\pi (h - f)T)}{2\pi (h - f)T} + \frac{\sin(2\pi (h + f)T)}{2\pi (h + f)T}, & \text{otherwise.} \end{cases}$$

$$\Rightarrow \lim_{T \to \infty} \left(\frac{1}{T} \int_{-T}^{T} s(t) \cdot e^{-2\pi i f t} dt \right) = \begin{cases} 1, & \text{if } f = h, \\ 0, & \text{otherwise.} \end{cases}$$

So, the transform can detect if f = h!

Noise Reduction



Source: http://www.mediacy.com/index.aspx?page=AH_FFTExample

Data Compression

- Discrete Cosine Transforms (DCT) are used for lossy data compression (e.g., MP3, JPEG, MPEG)
- DCT is a Fourier-related transform similar to DFT (Discrete Fourier Transform) but uses only real data (uses cosine waves only instead of both cosine and sine waves)
- Forward DCT transforms data from spatial to frequency domain
- Each frequency component is represented using a fewer number of bits (i.e., truncated / quantized)
- Low amplitude high frequency components are also removed
- Inverse DCT then transforms the data back to spatial domain
- The resulting image compresses better

Data Compression

Transformation to frequency domain using cosine transforms work in the same way as the Fourier transform.

Suppose: $s(t) = \cos(2\pi h \cdot t)$

$$\frac{1}{T} \int_{-T}^{T} s(t) \cdot \cos(2\pi f t) dt = \begin{cases} 1 + \frac{\sin(4\pi f T)}{4\pi f T}, & \text{if } f = h, \\ \frac{\sin(2\pi (h - f)T)}{2\pi (h - f)T} + \frac{\sin(2\pi (h + f)T)}{2\pi (h + f)T}, & \text{otherwise.} \end{cases}$$

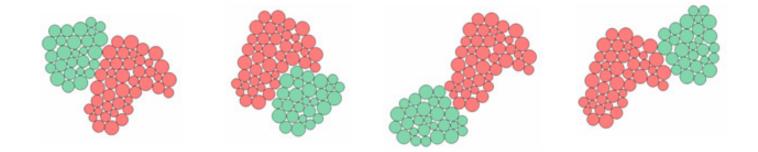
$$\Rightarrow \lim_{T \to \infty} \left(\frac{1}{T} \int_{-T}^{T} s(t) \cdot \cos(2\pi f t) \, dt \right) = \begin{cases} 1, & \text{if } f = h, \\ 0, & \text{otherwise.} \end{cases}$$

So, this transform can also detect if f = h.

Protein-Protein Docking

- ☐ Knowledge of complexes is used in
 - Drug design

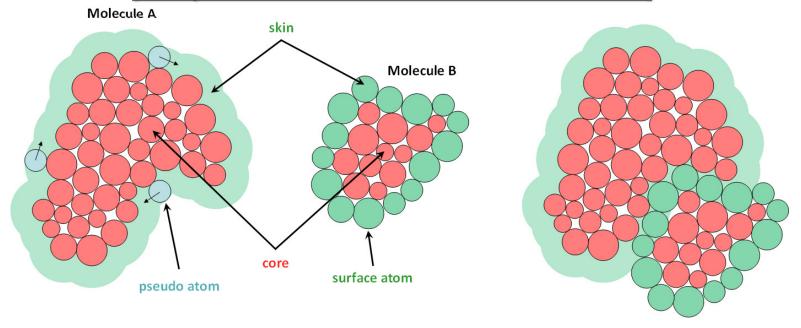
- Structure function analysis
- Studying molecular assemblies Protein interactions
- ☐ Protein-Protein Docking: Given two proteins, find the best relative transformation and conformations to obtain a stable complex.



- ☐ Docking is a hard problem
 - Search space is huge (6D for rigid proteins)
 - Protein flexibility adds to the difficulty

Shape Complementarity

<u>[Wang'91, Katchalski-Katzir et al.'92, Chen et al.'03]</u>



a possible docking solution

To maximize skin-skin overlaps and minimize core-core overlaps

- assign positive real weights to skin atoms
- assign positive imaginary weights to core atoms

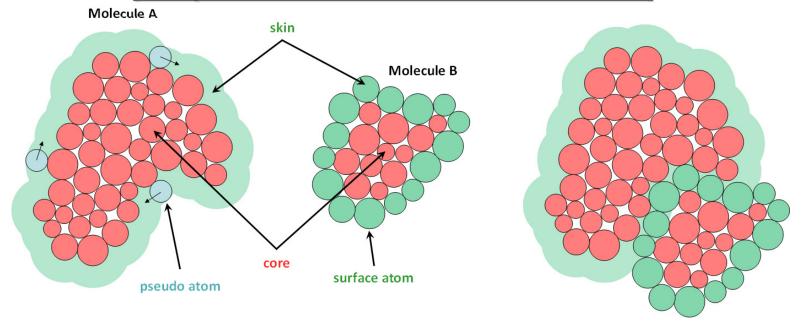
Let A 'denote molecule A with the pseudo skin atoms.

For $P \in \{A', B\}$ with M_P atoms, affinity function: $f_P(x) = \sum_{k=1}^{M_P} w_k \cdot g_k(x)$

Here $g_k(x)$ is a Gaussian representation of atom k, and w_k its weight.

Shape Complementarity

[Wang'91, Katchalski-Katzir et al.'92, Chen et al.'03]



a possible docking solution

Let A 'denote molecule A with the pseudo skin atoms.

For $P \in \{A', B\}$ with M_P atoms, affinity function:

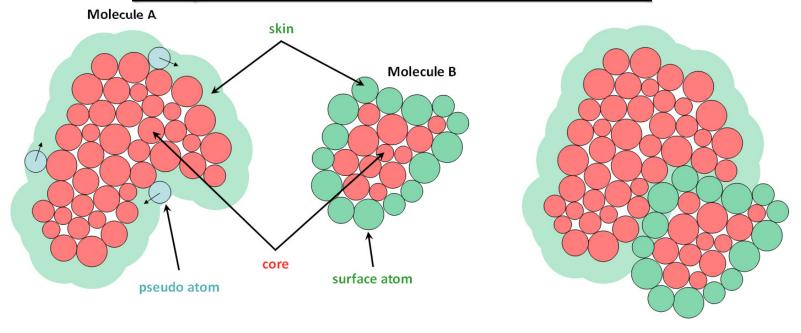
$$f_P(x) = \sum_{k=1}^{M_P} w_k \cdot g_k(x)$$

For rotation r and translation t of molecule B (i.e., $B_{t,r}$),

the interaction score, $F_{A,B}(t,r) = \int_{x} f_{A'}(x) f_{B_{t,r}}(x) dx$

Shape Complementarity

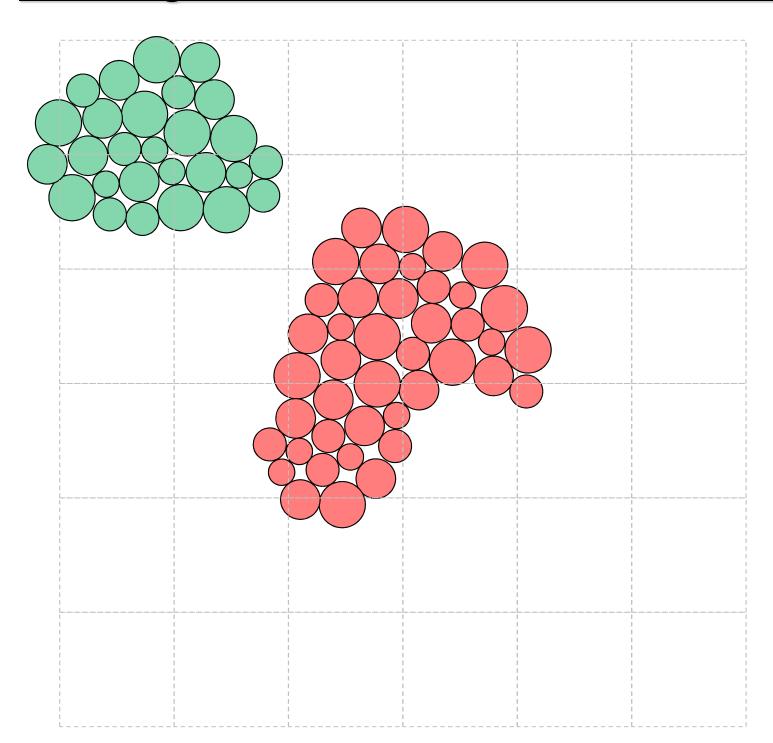
[Wang'91, Katchalski-Katzir et al.'92, Chen et al.'03]

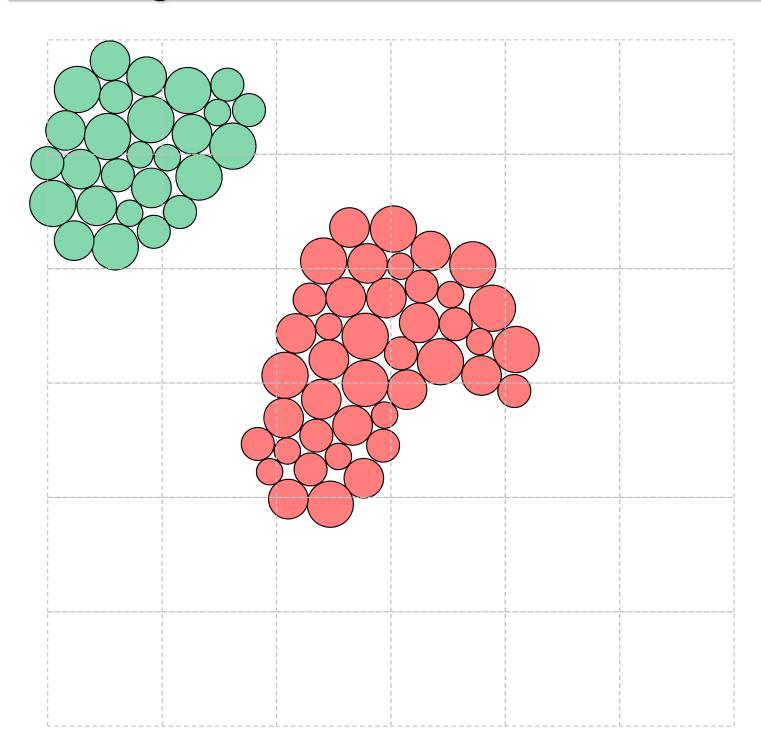


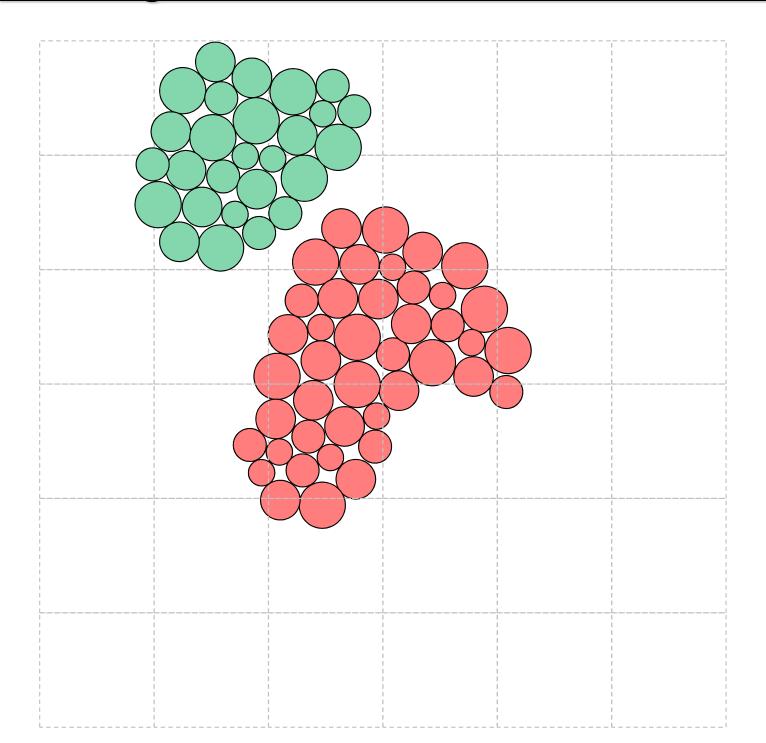
a possible docking solution

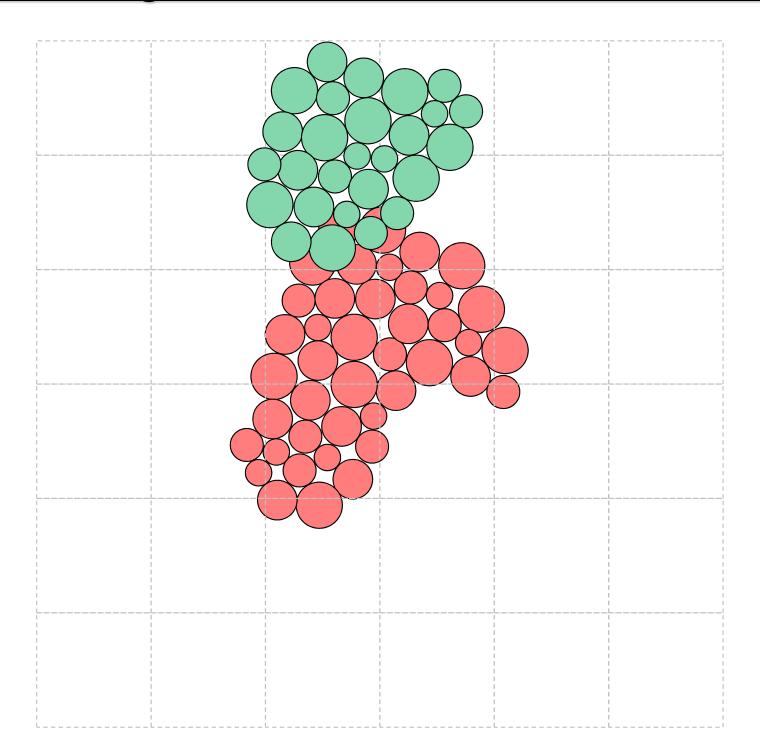
For rotation r and translation t of molecule B (i.e., $B_{t,r}$), the interaction score, $F_{A,B}(t,r) = \int_x f_{A'}(x) f_{B_{t,r}}(x) dx$

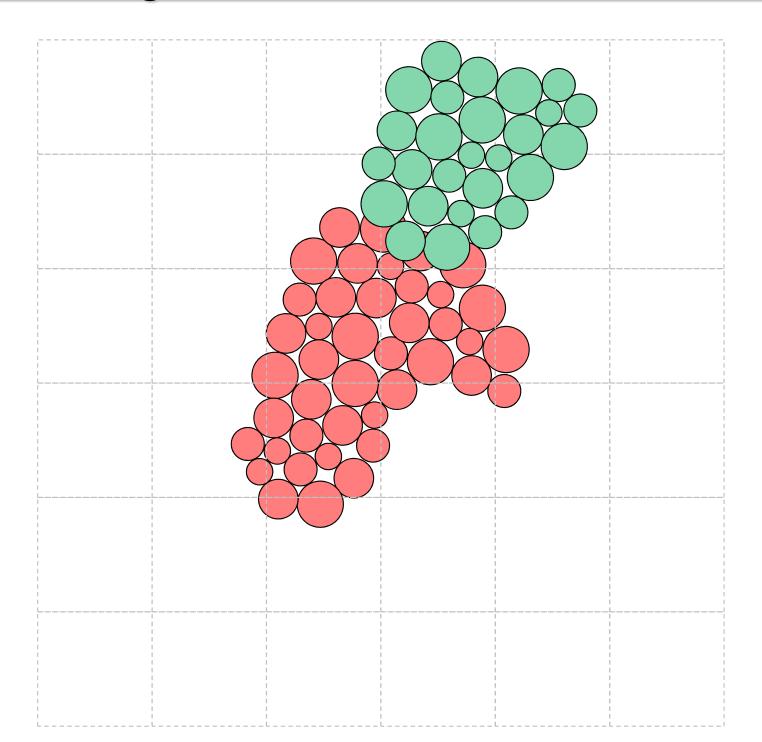
 $Re\left(F_{A,B}(t,r)\right)=$ skin-skin overlap score – core-core overlap score $Im\left(F_{A,B}(t,r)\right)=$ skin-core overlap score

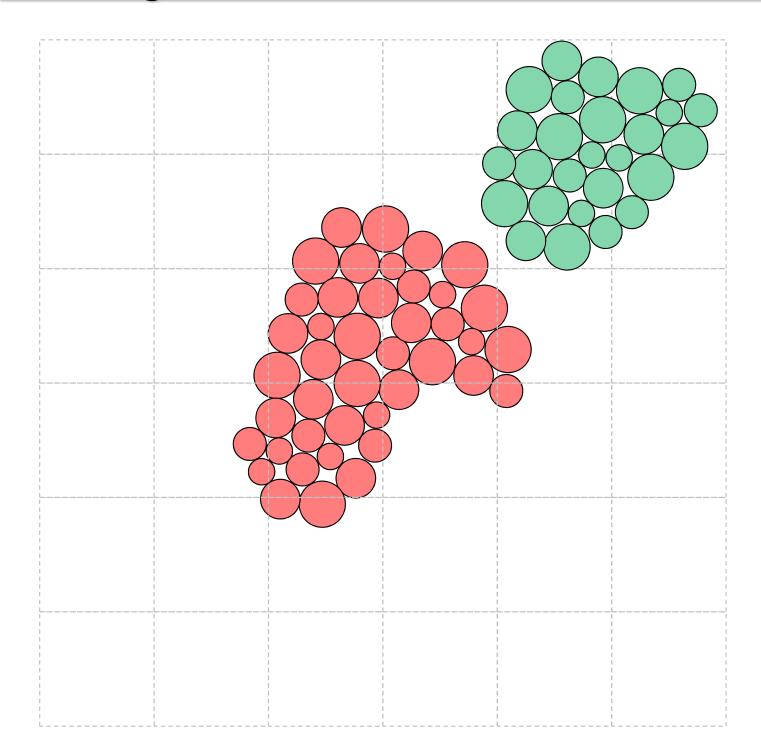


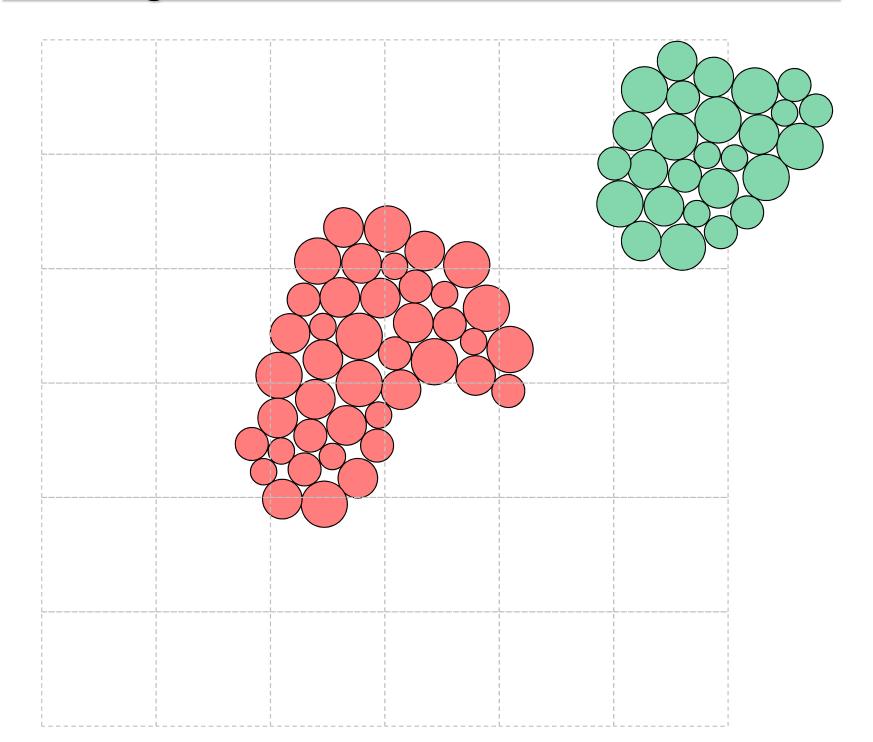


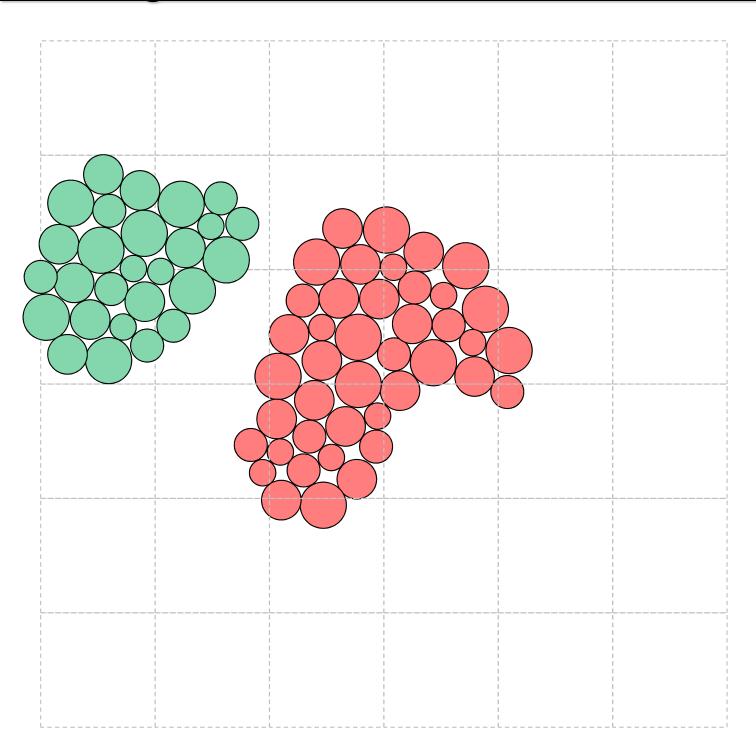


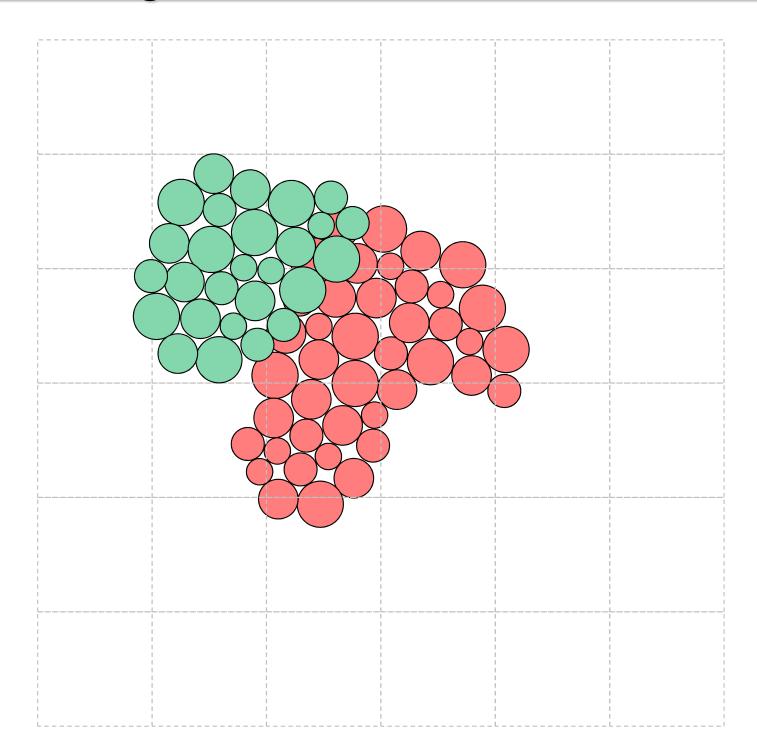


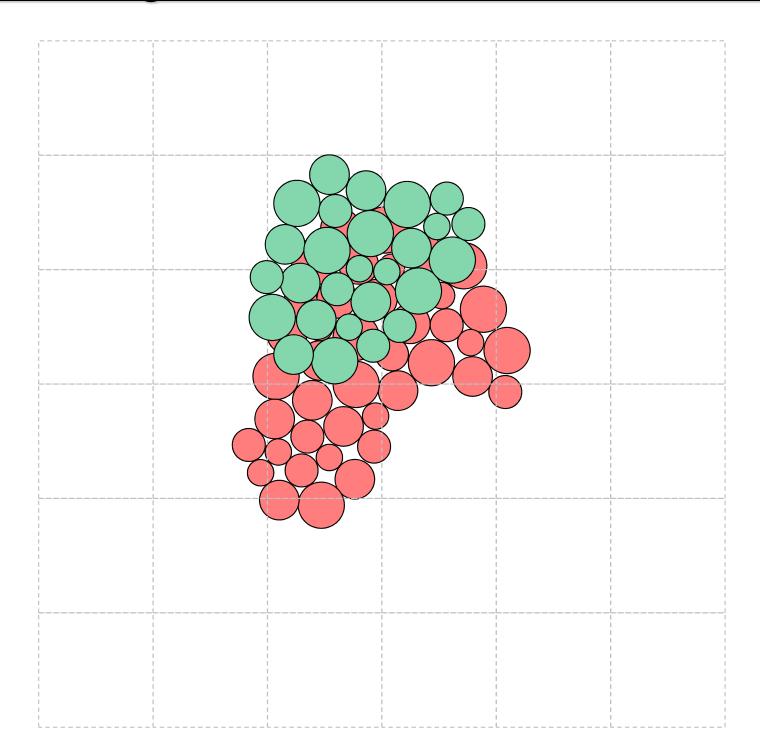


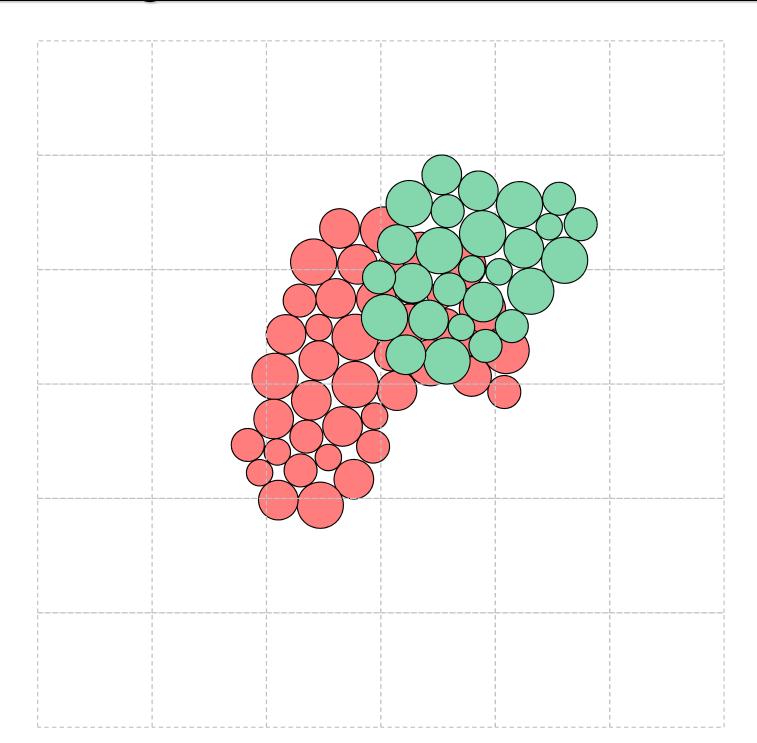


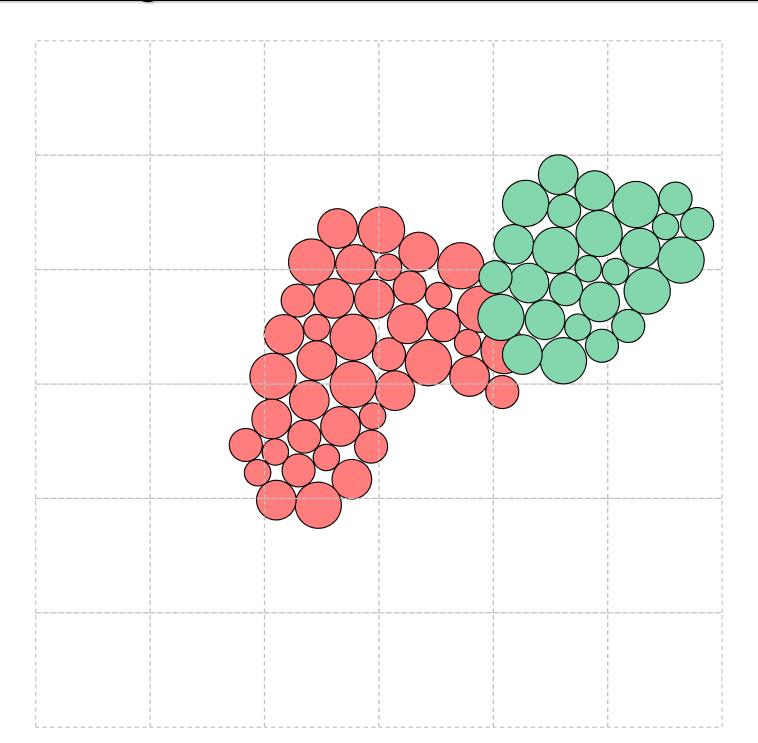


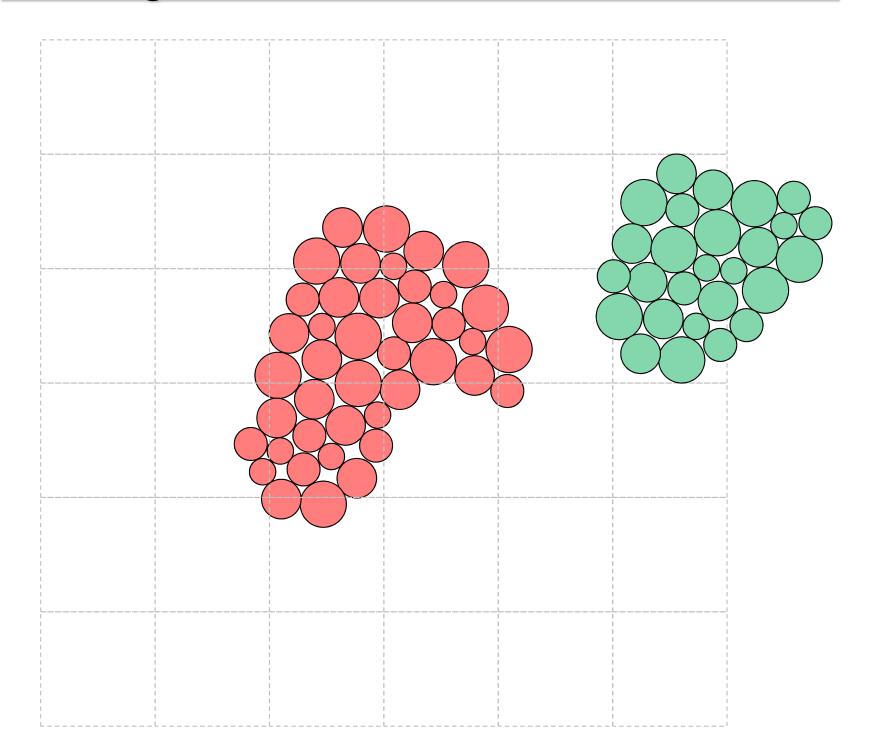


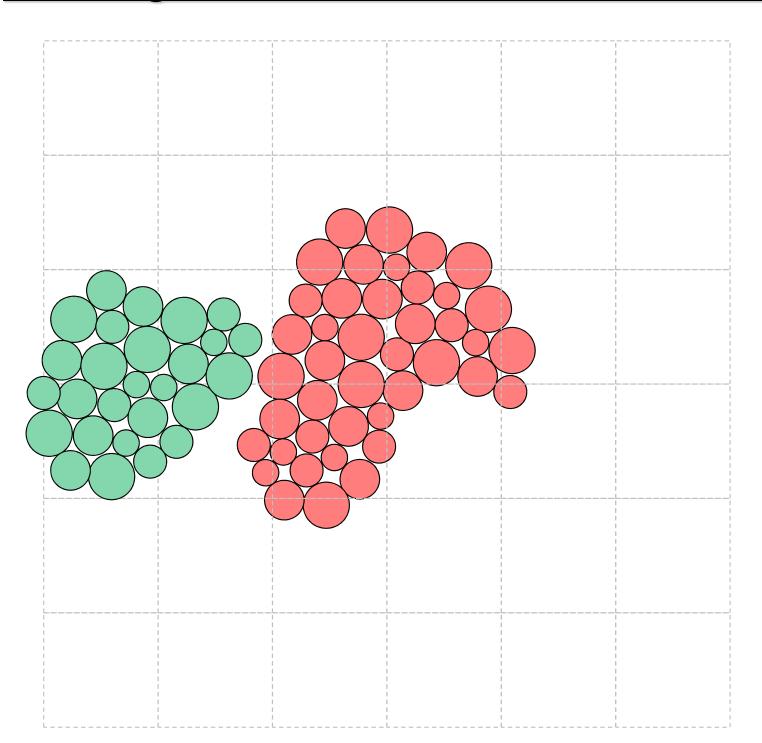


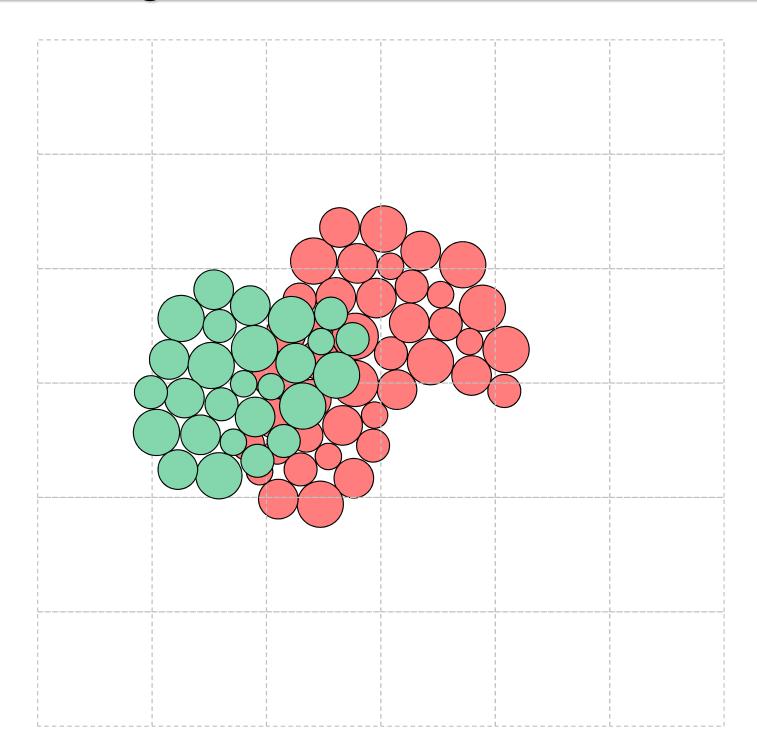


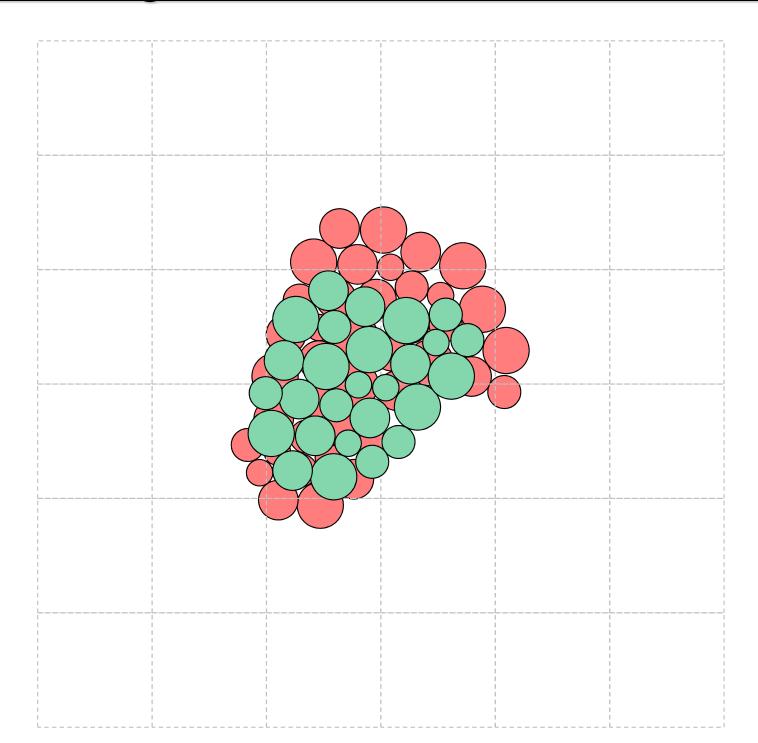


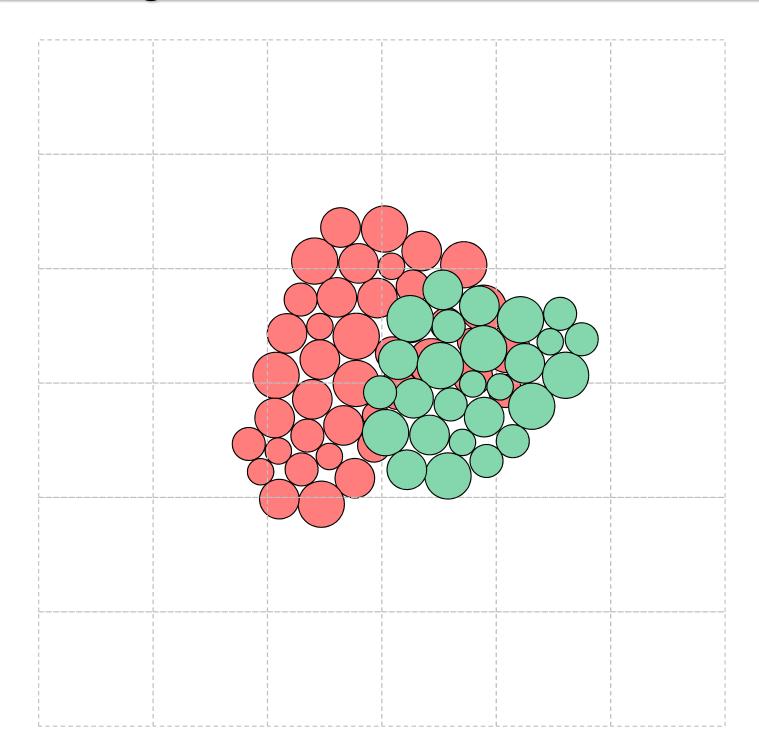


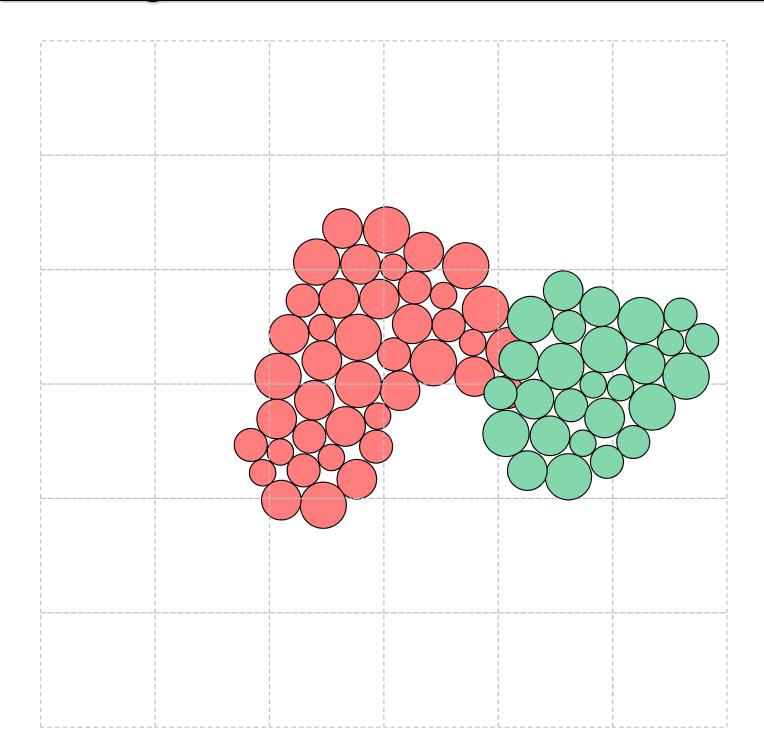


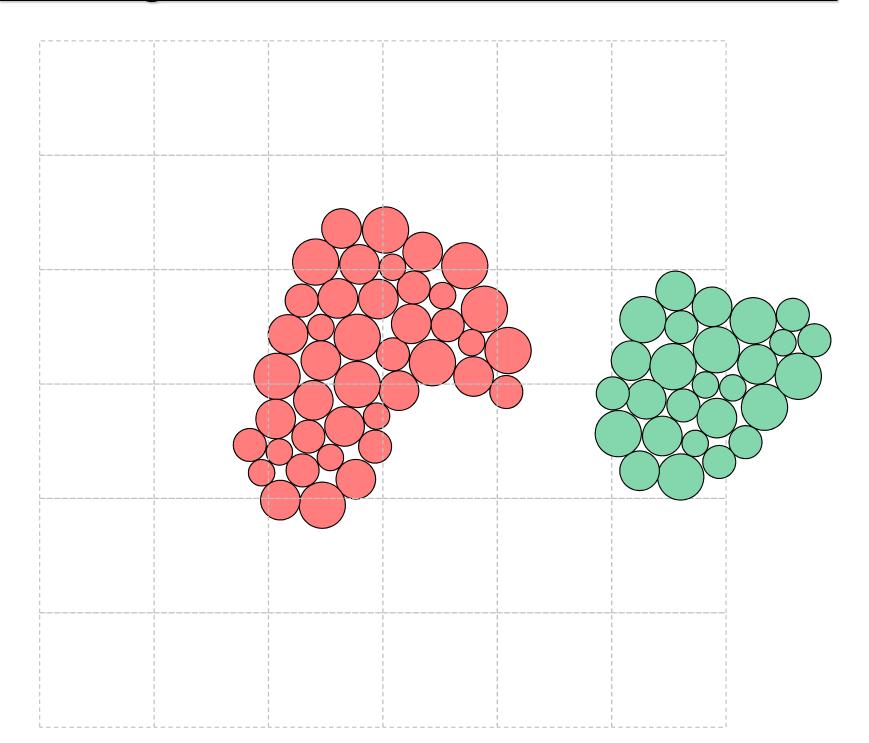


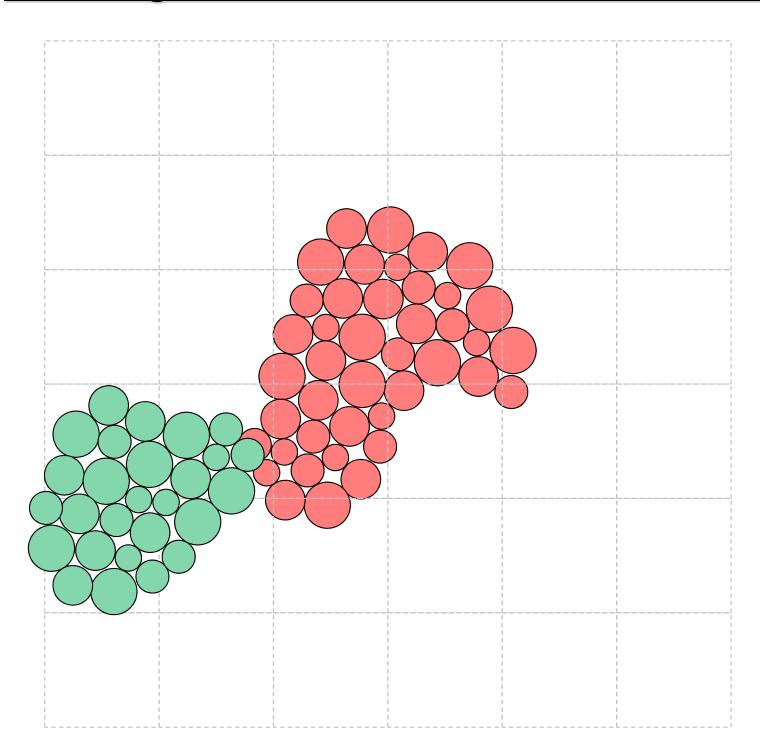


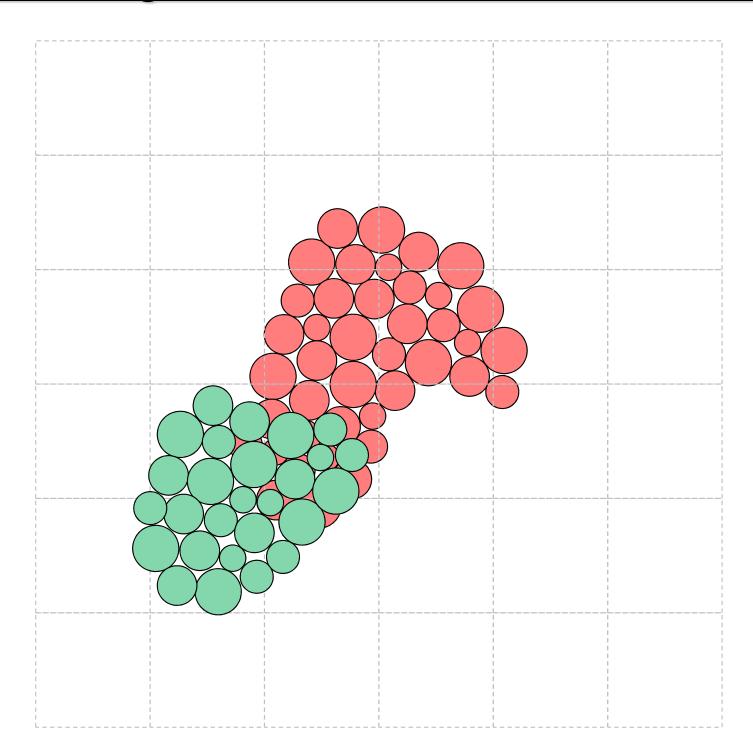


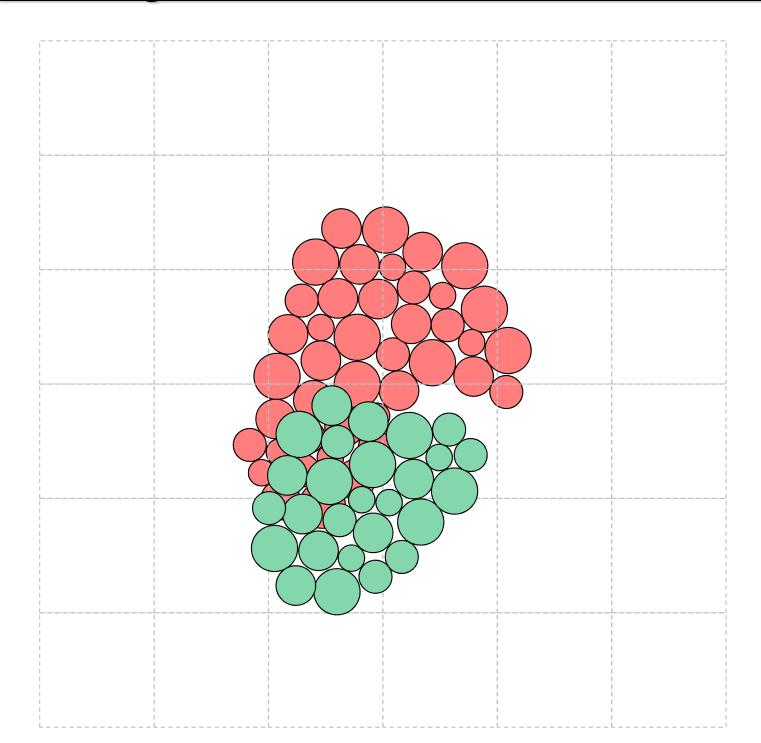


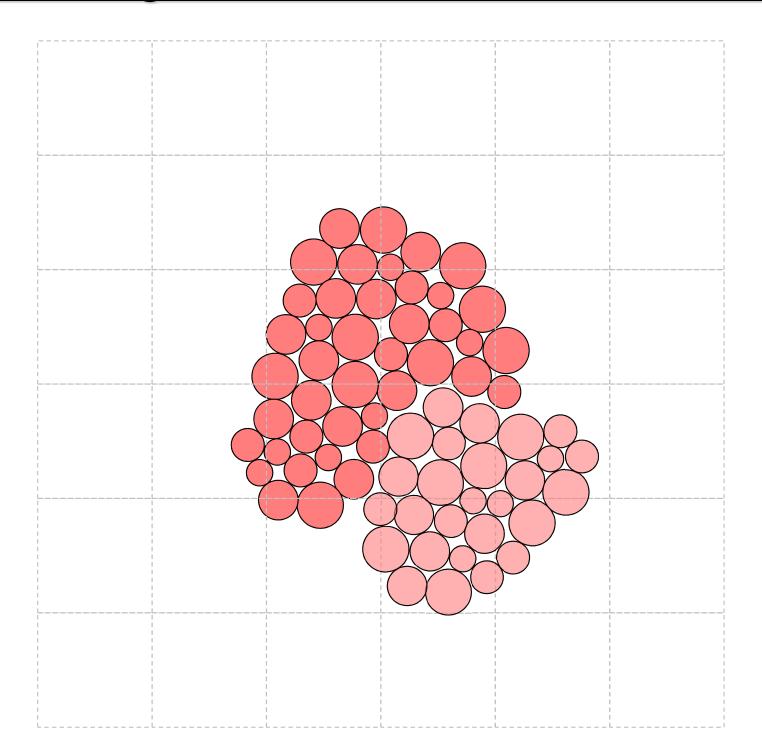


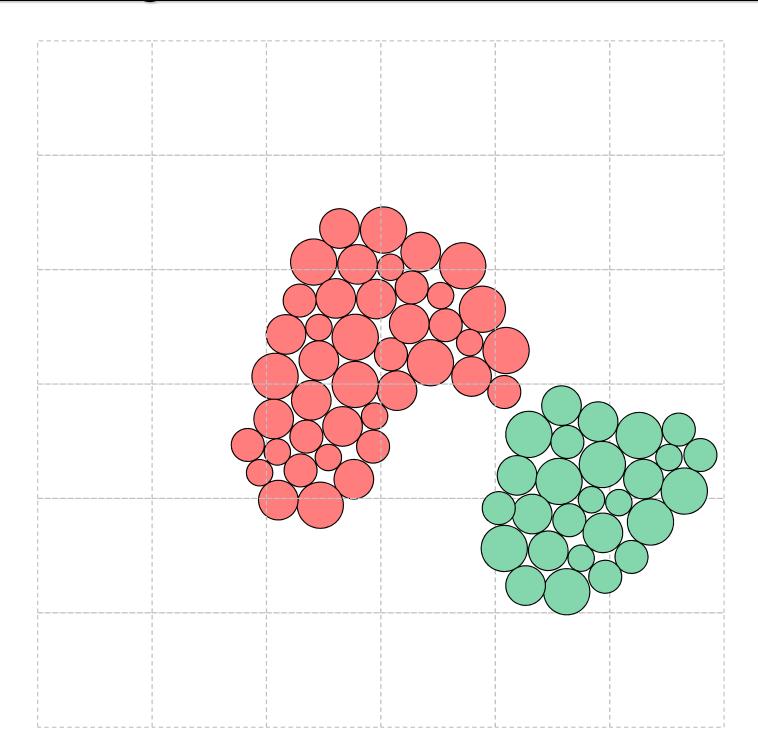


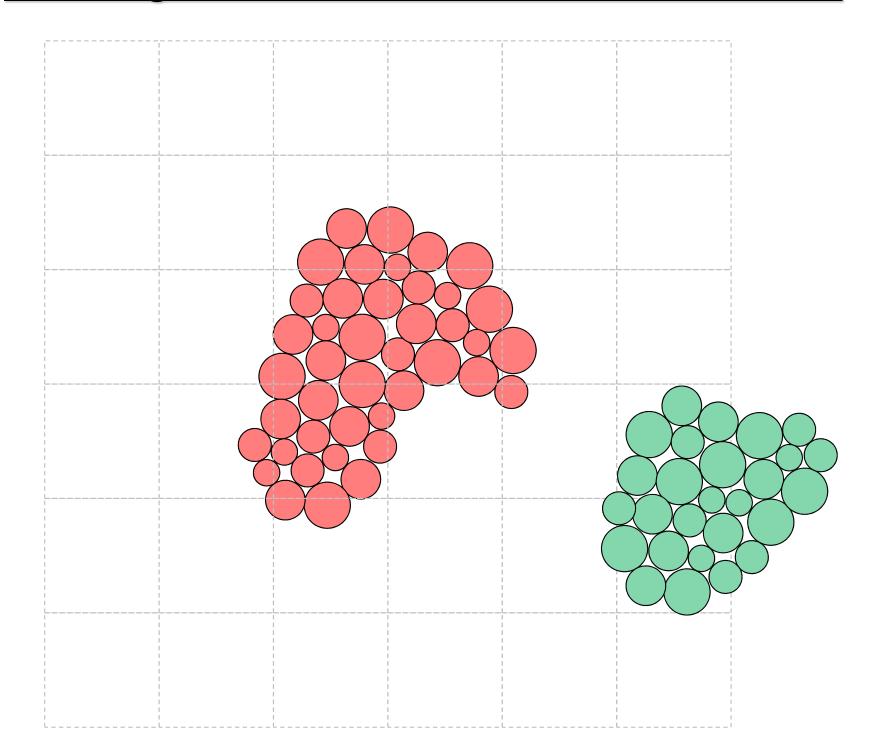


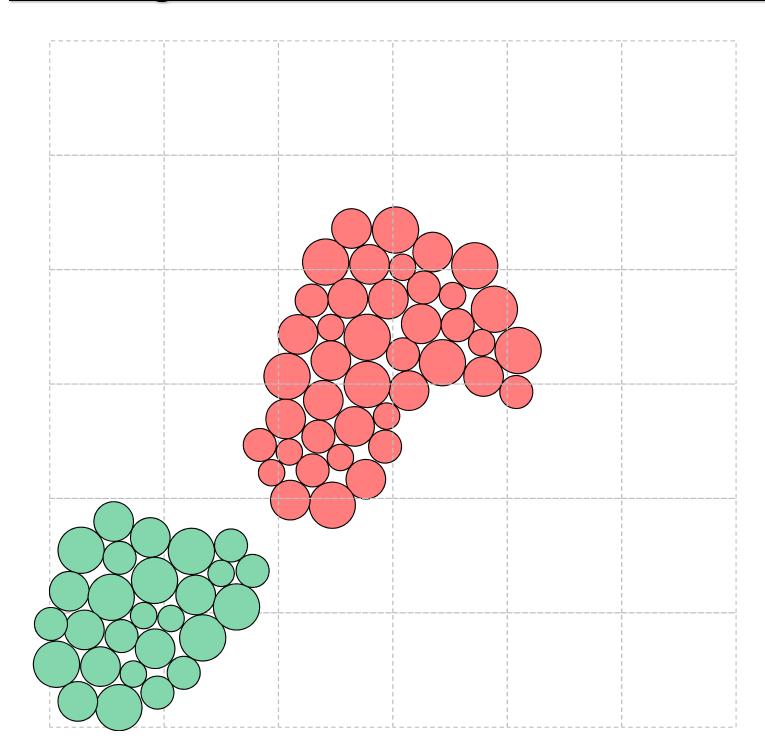


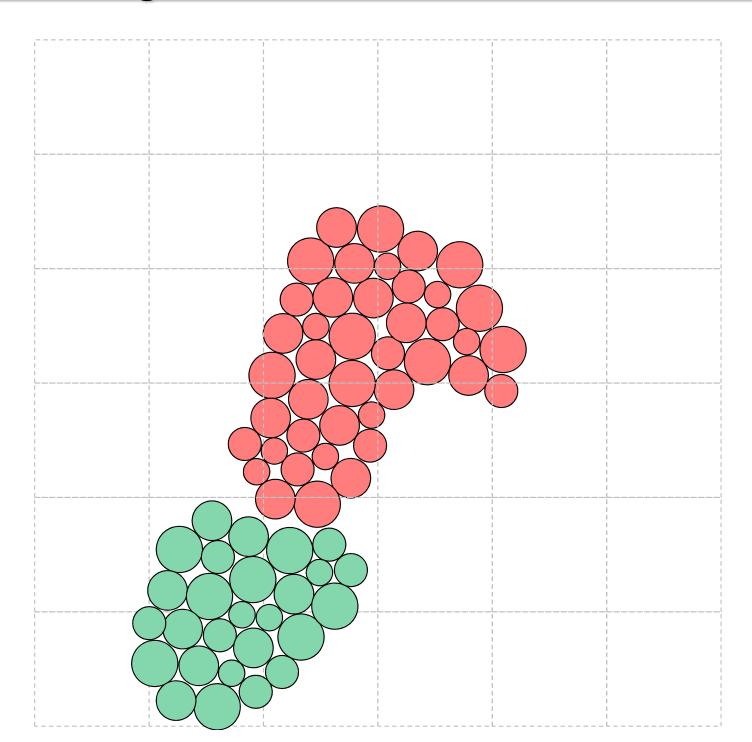


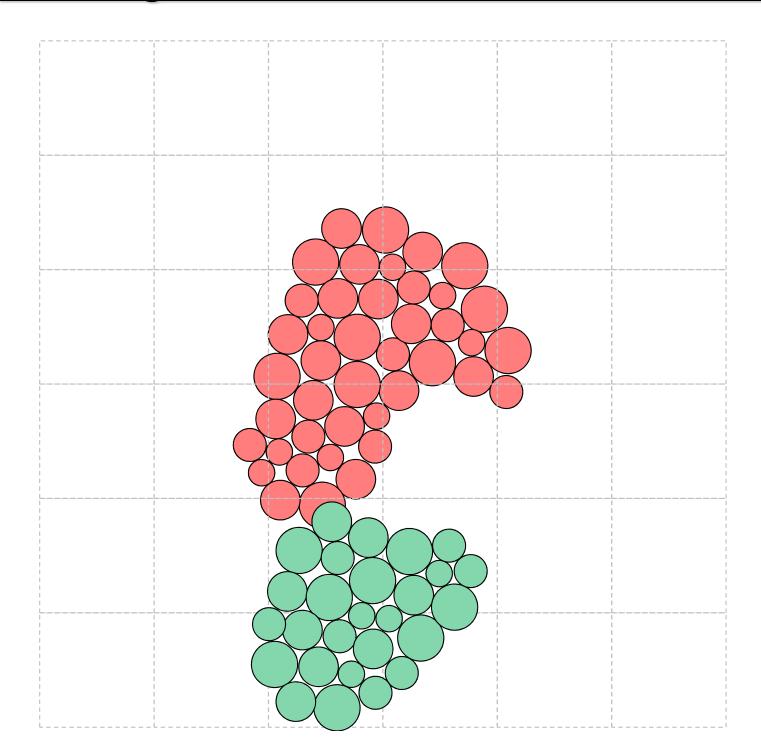


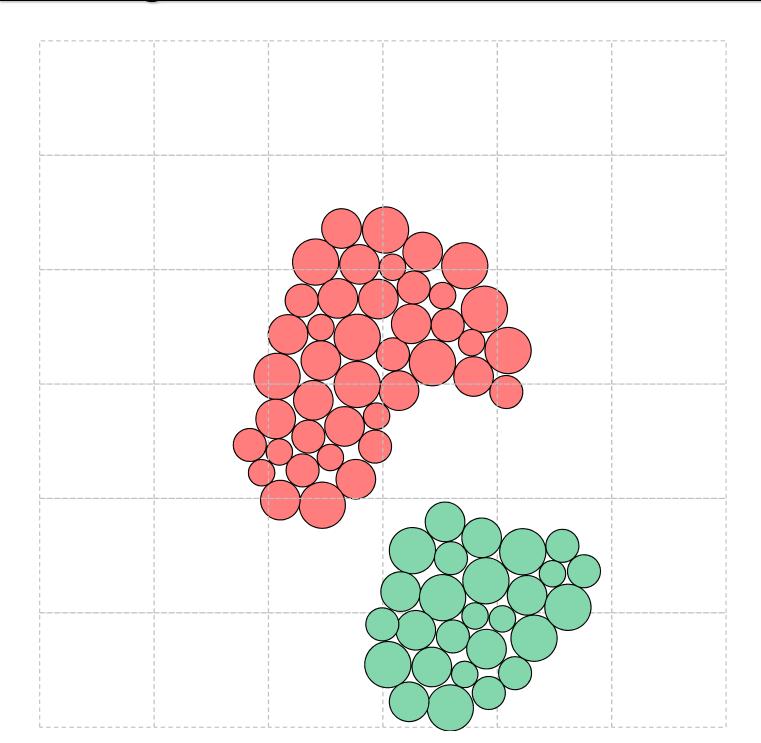


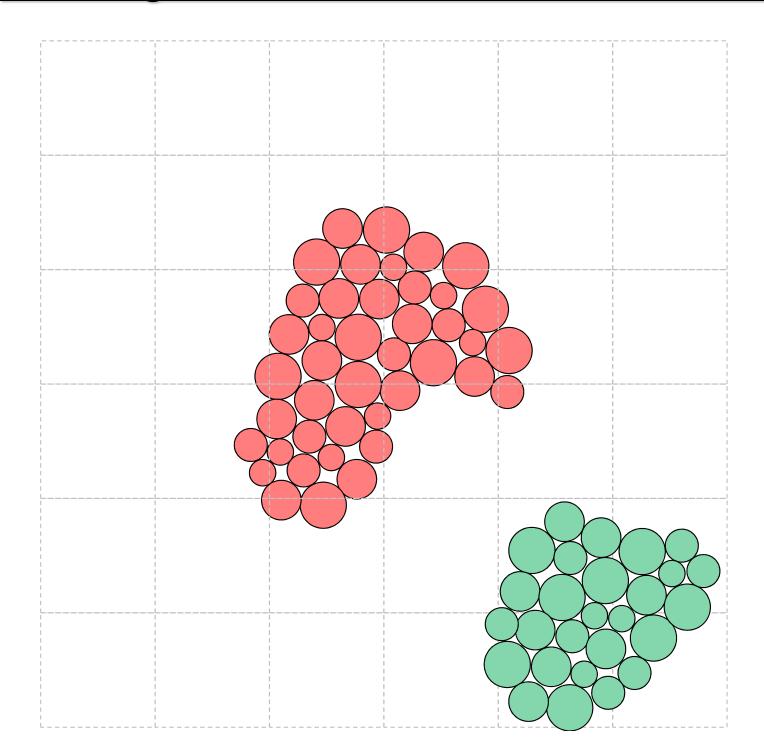


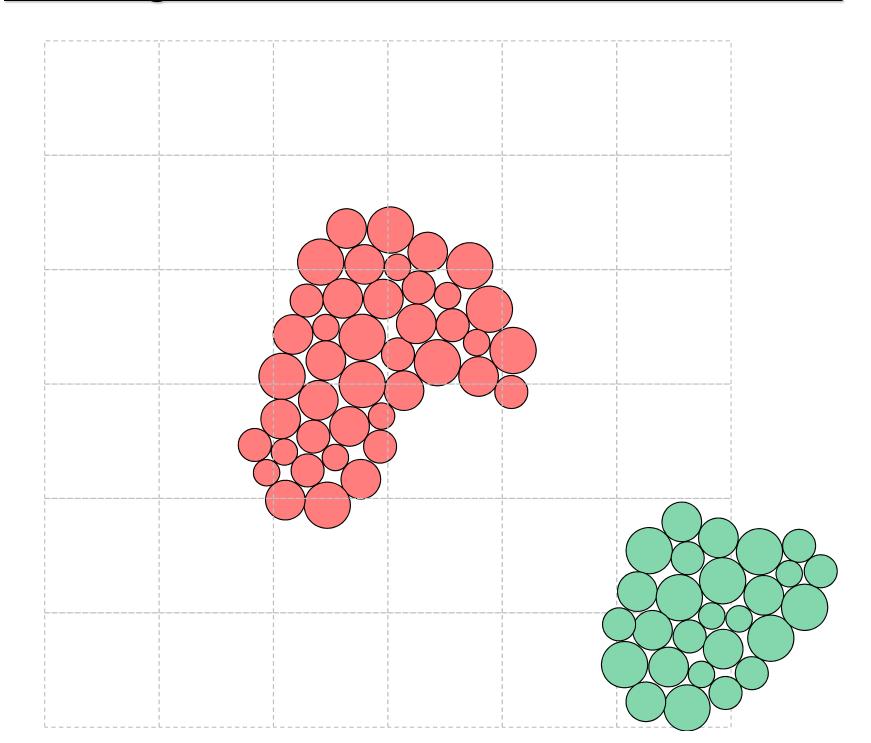




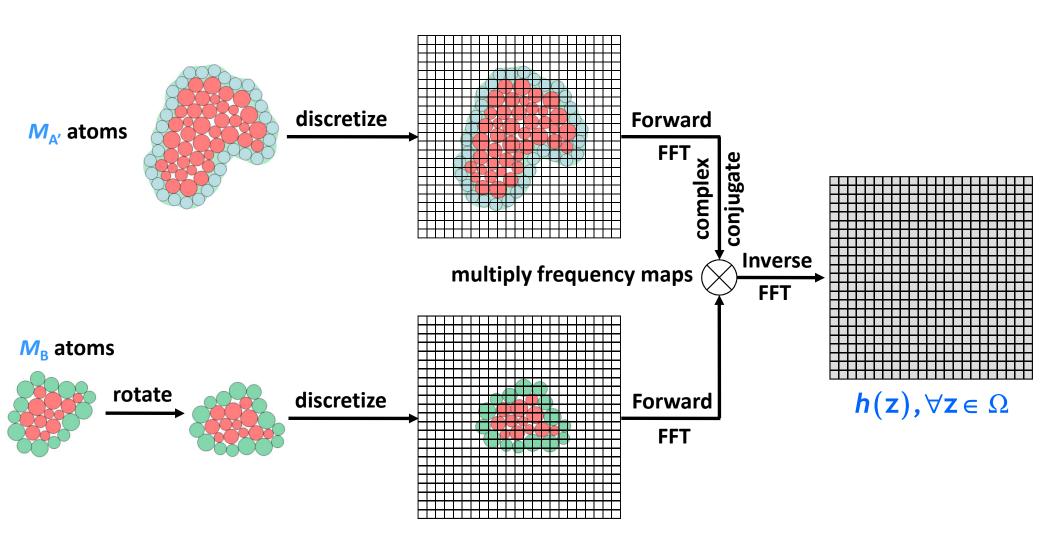








<u>Translational Search using FFT</u>



$$\forall z \in \Omega = [-n, n]^3, \qquad h(z) = \int_{x \in \Omega} f_{A'}(x) f_{B_r}(z - x) dx$$

