CSE 548: Analysis of Algorithms

Lecture 5
(Divide-and-Conquer Algorithms: Polynomial Multiplication (Continued))

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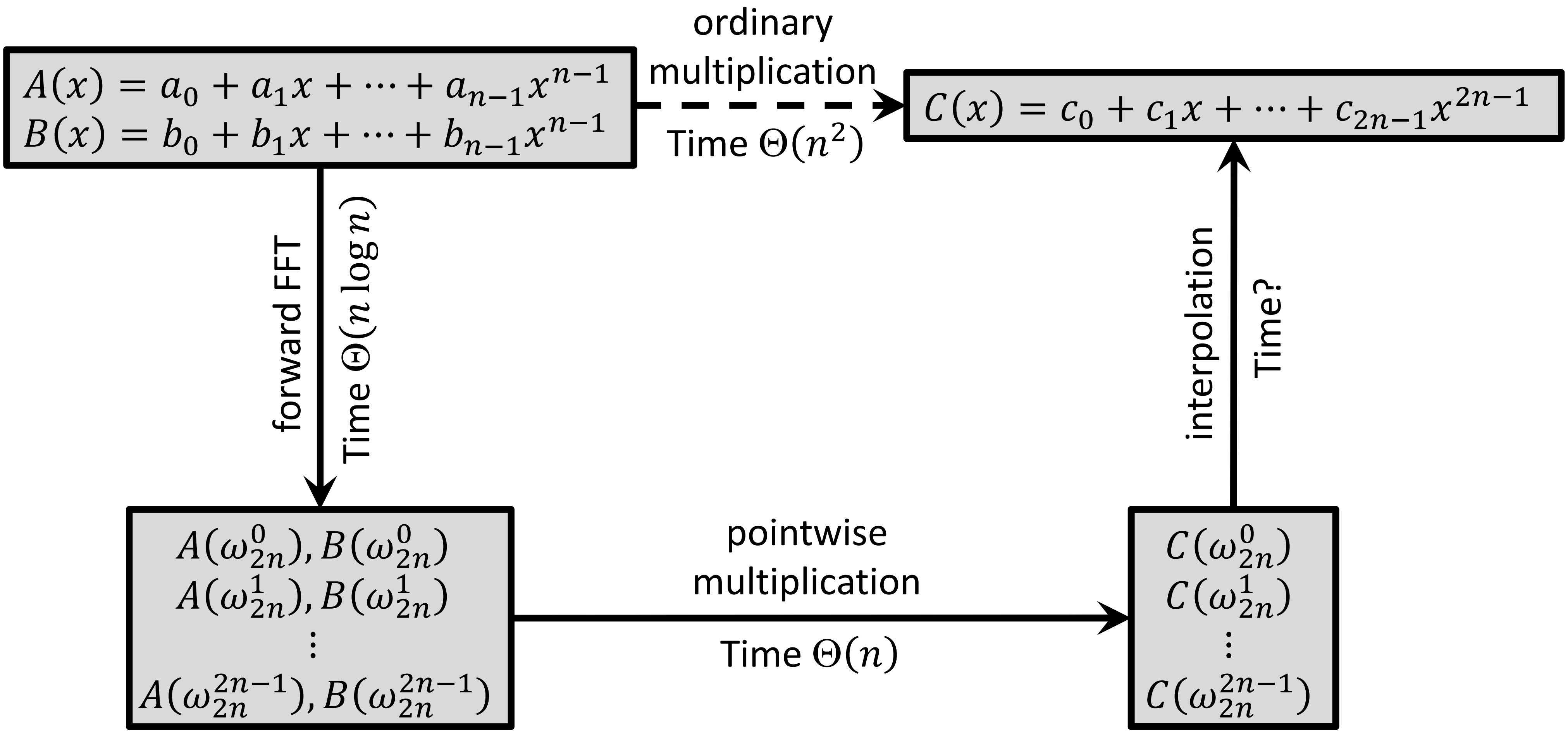
Faster Polynomial Multiplication?
(in Coefficient Form)



Point-Value Form $\Rightarrow$ Coefficient Form

Given: $$\underbrace{\begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega_n & (\omega_n)^2 & \cdots & (\omega_n)^{n-1} \\ 1 & \omega_n^2 & (\omega_n^2)^2 & \cdots & (\omega_n^2)^{n-1} \\ . & . & . & \cdots & . \\ . & . & . & \cdots & . \\ 1 & \omega_n^{n-1} & (\omega_n^{n-1})^2 & \cdots & (\omega_n^{n-1})^{n-1} \end{bmatrix}}_{\substack{V(\omega_n) \\ Vandermonde\ Matrix}} \underbrace{\begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ . \\ . \\ a_{n-1} \end{bmatrix}}_{\bar{a}} = \underbrace{\begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ . \\ . \\ y_{n-1} \end{bmatrix}}_{\bar{y}}$$

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

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

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

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

Point-Value Form $\Rightarrow$ Coefficient Form

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 $0 \leq j, k \leq n-1$, the $(j,k)^{th}$ entries are:

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

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

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

Point-Value Form $\Rightarrow$ Coefficient Form

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

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 $p \neq q$:

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

$$= \frac{1}{n} \times \frac{(\omega_n^{n})^{q-p} - 1}{\omega_n^{q-p} - 1} = \frac{1}{n} \times \frac{(1)^{q-p} - 1}{\omega_n^{q-p} - 1} = 0$$

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

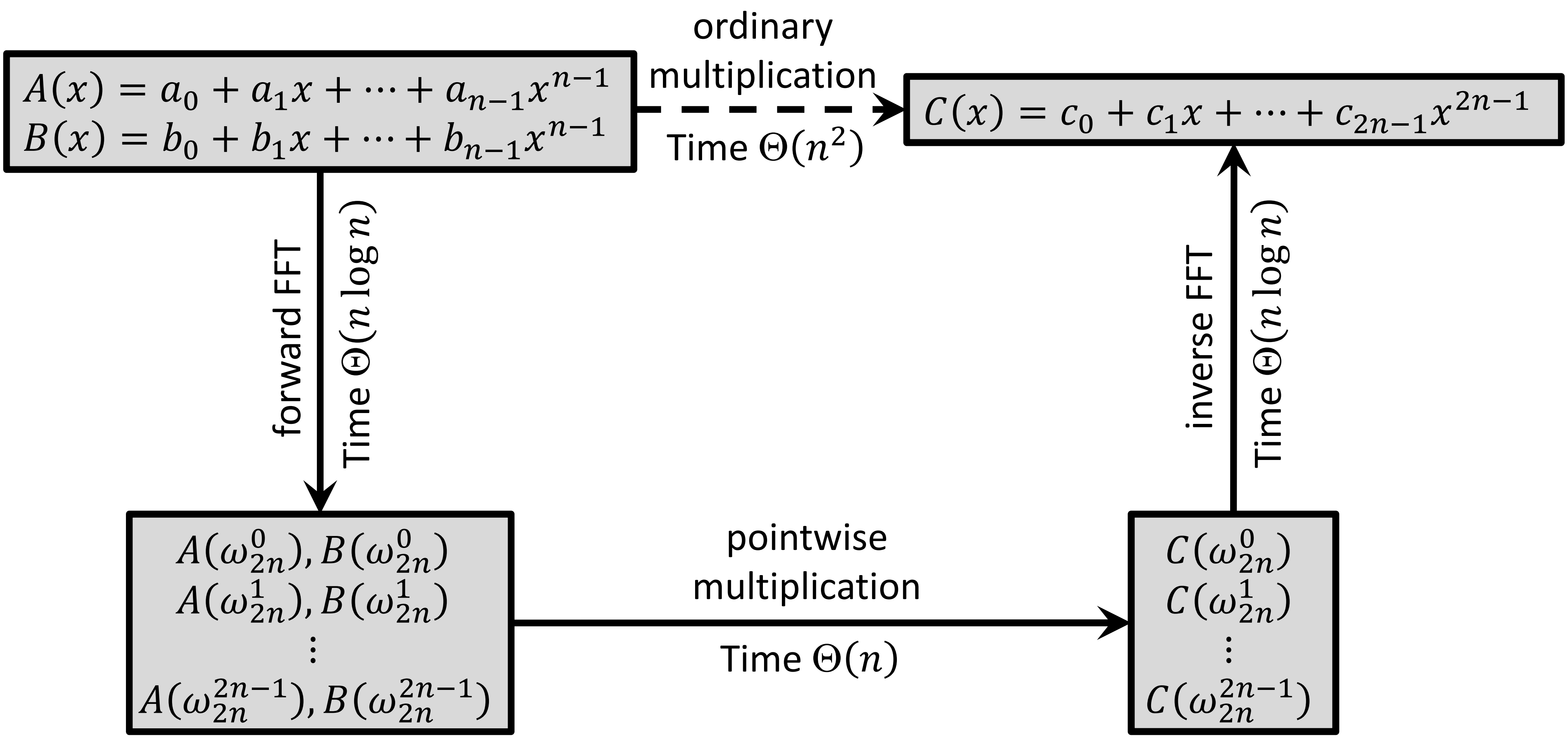
Point-Value Form ⇒ Coefficient Form

We need to compute the following matrix-vector product:

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

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!

Faster Polynomial Multiplication? (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

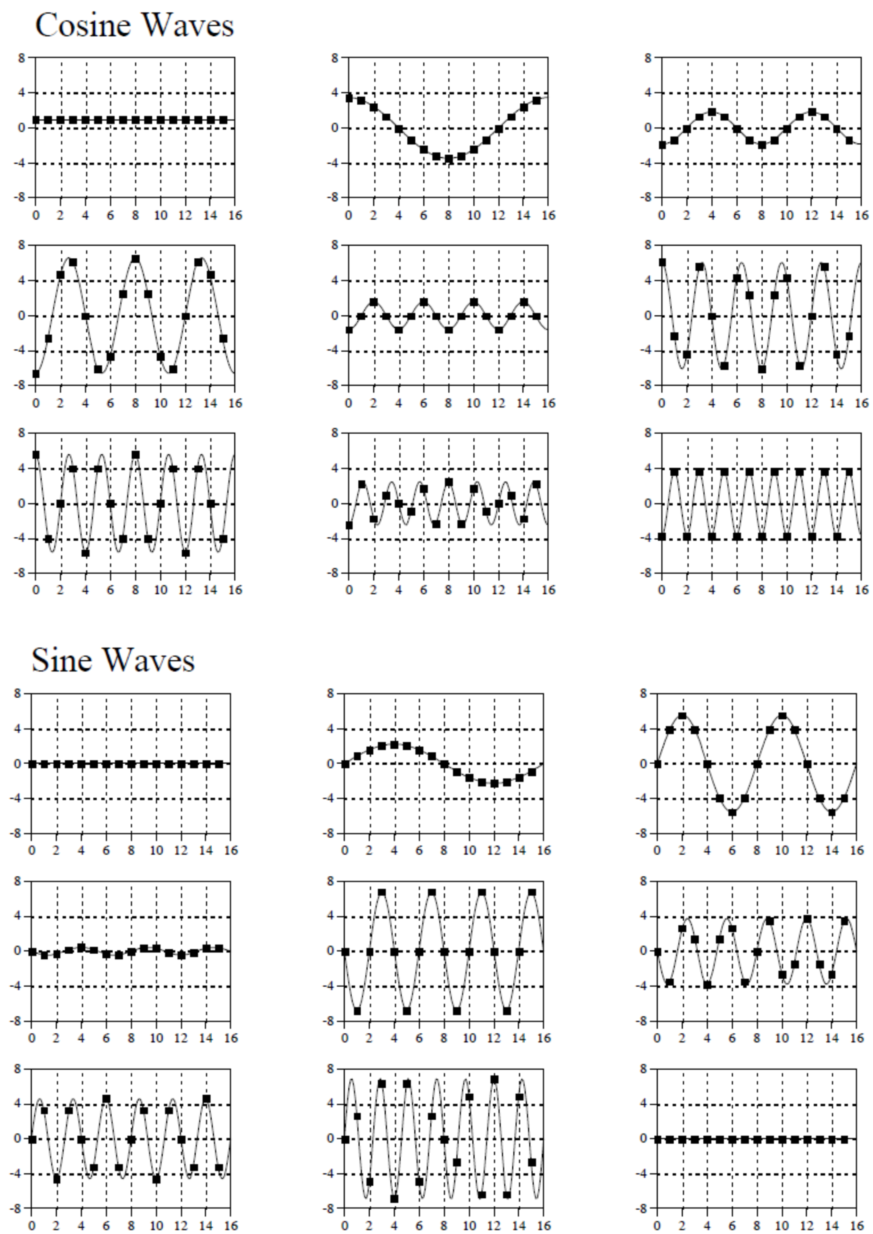
Some Applications of Fourier Transform and FFT

Jean Baptiste Joseph Fourier

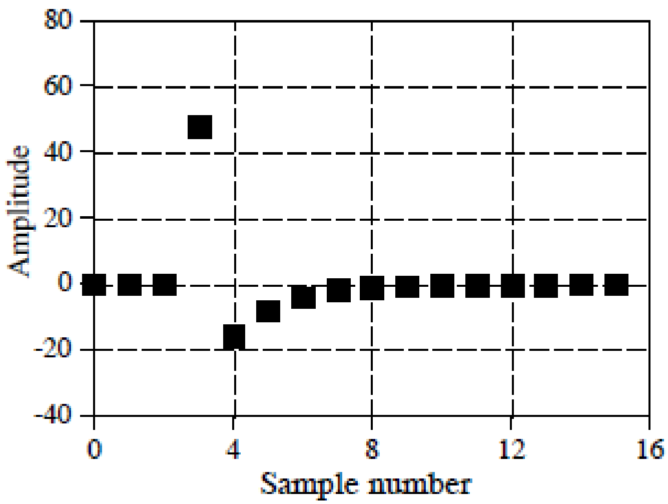
Any periodic signal can be represented as a sum of a series of sinusoidal (sine & cosine) waves. [1807]

Spatial (Time) Domain ⇔ Frequency Domain

Frequency Domain



Spatial (Time) Domain



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

Spatial (Time) Domain ⇔ Frequency Domain (Fourier Transforms)

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.

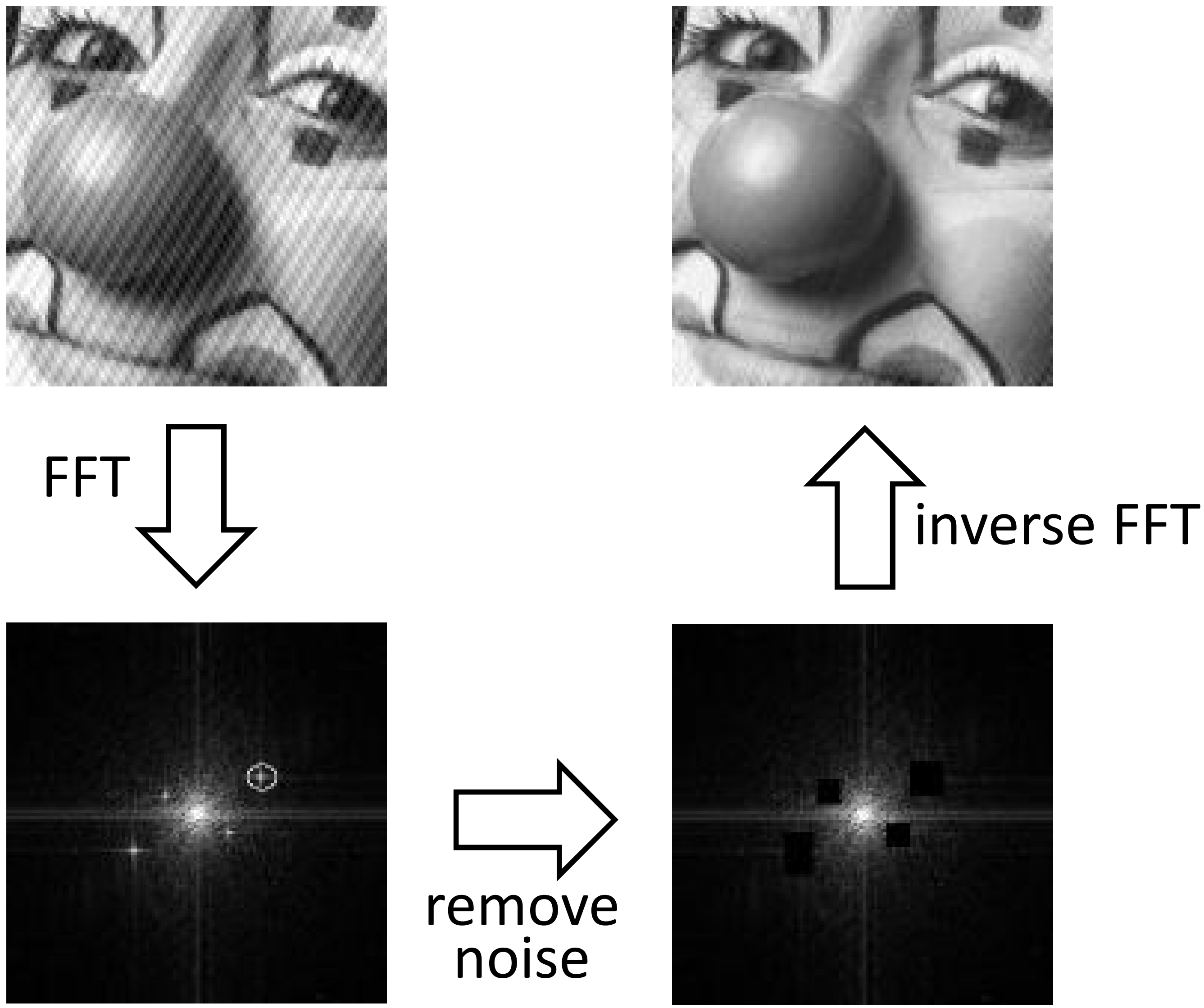
Suppose: $s(t) = \cos(2\pi h \cdot t)$

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

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

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

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

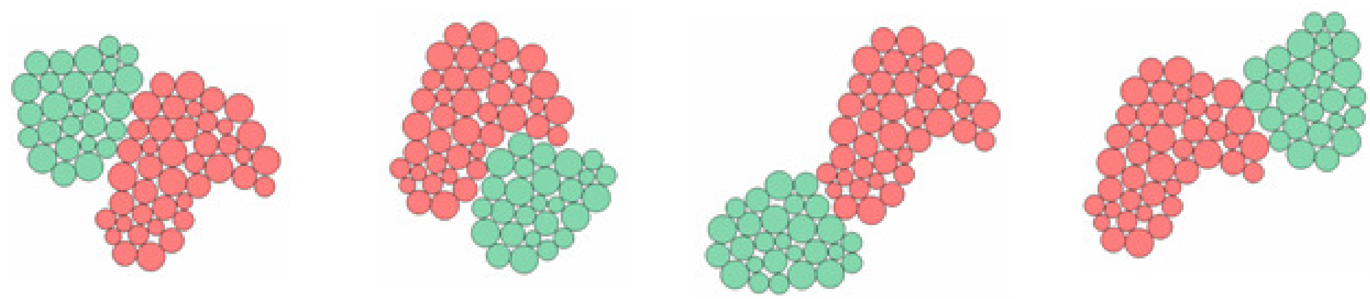
$$\Rightarrow \lim_{T\to\infty}\left(\frac{1}{T}\int_{-T}^{T} s(t) \cdot \cos(2\pi f t)\, dt\right) = \begin{cases} 1, & \text{if } f = h, \\ 0, & \text{otherwise.} \end{cases}$$

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

Protein-Protein Docking

- Knowledge of complexes is used in
  - Drug design
  - Studying molecular assemblies
  - Structure function analysis
  - Protein interactions

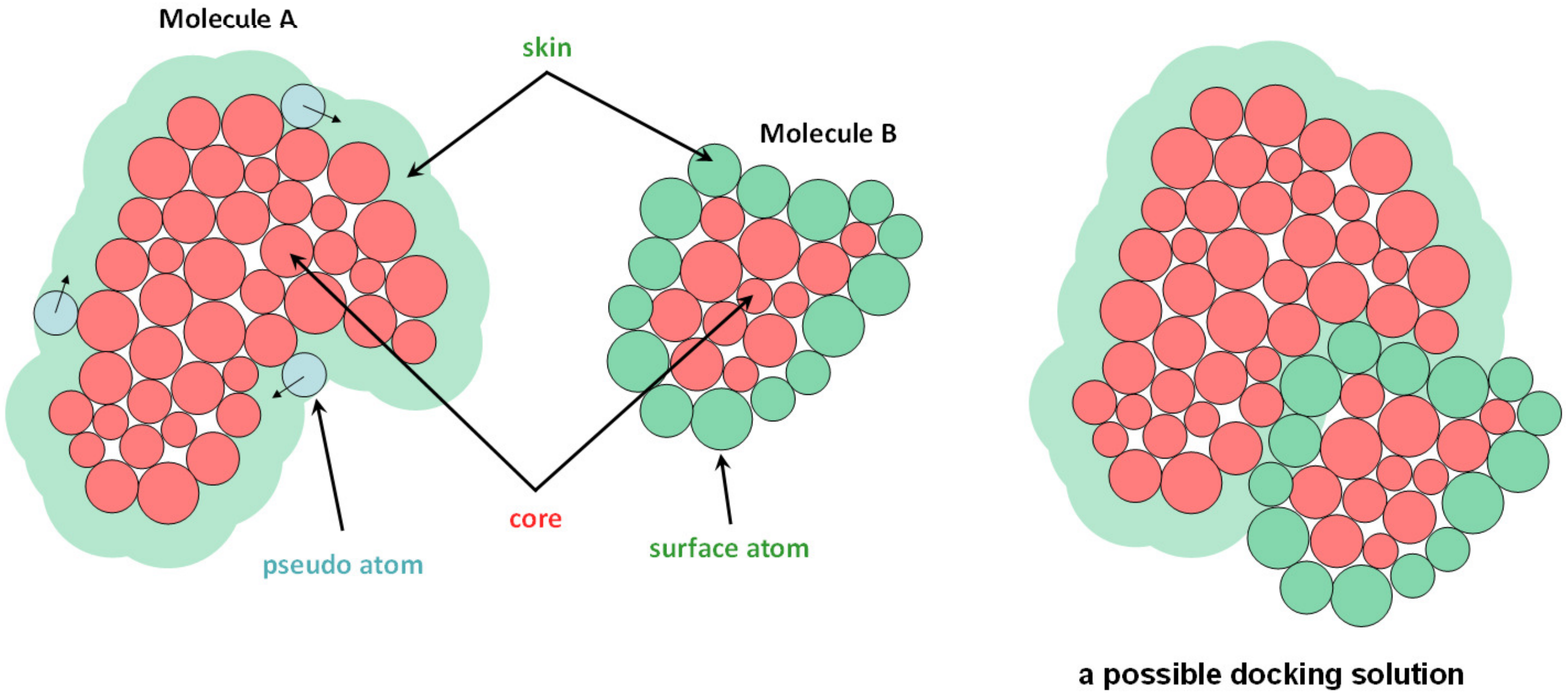
- Protein-Protein Docking: Given two proteins, find the best relative transformation and conformations to obtain a stable complex.



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

Shape Complementarity

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



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

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

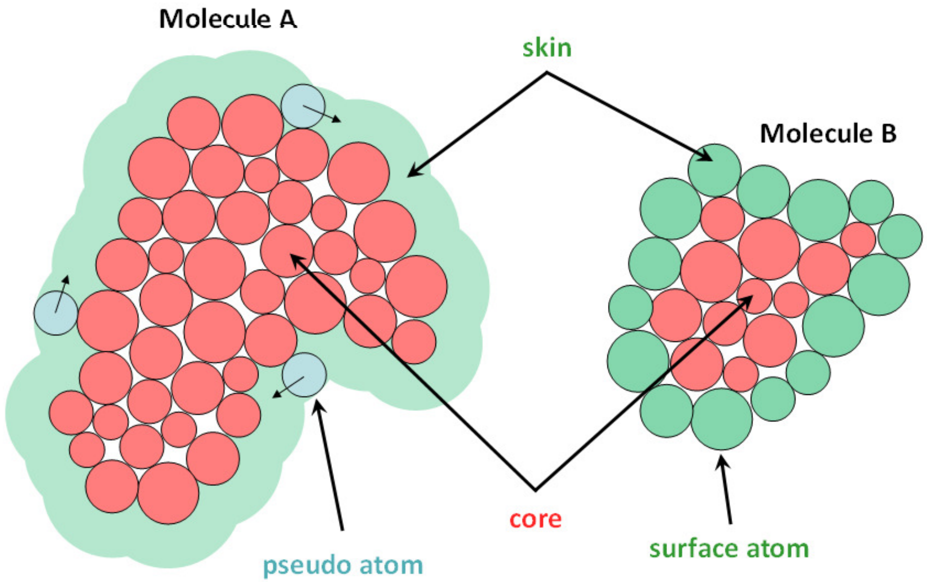
Let A' denote molecule A with the pseudo skin atoms.

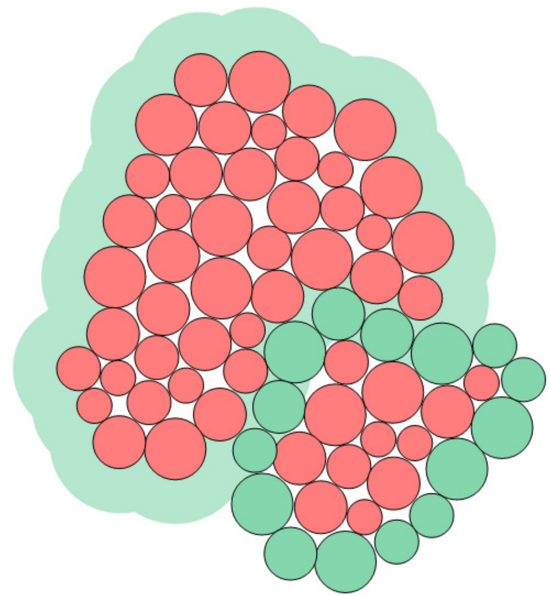
For $P \in \{A', B\}$ with M_P atoms, affinity function: $f_P(x) = \sum_{k=1}^{M_P} w_k \cdot g_k(x)$

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:

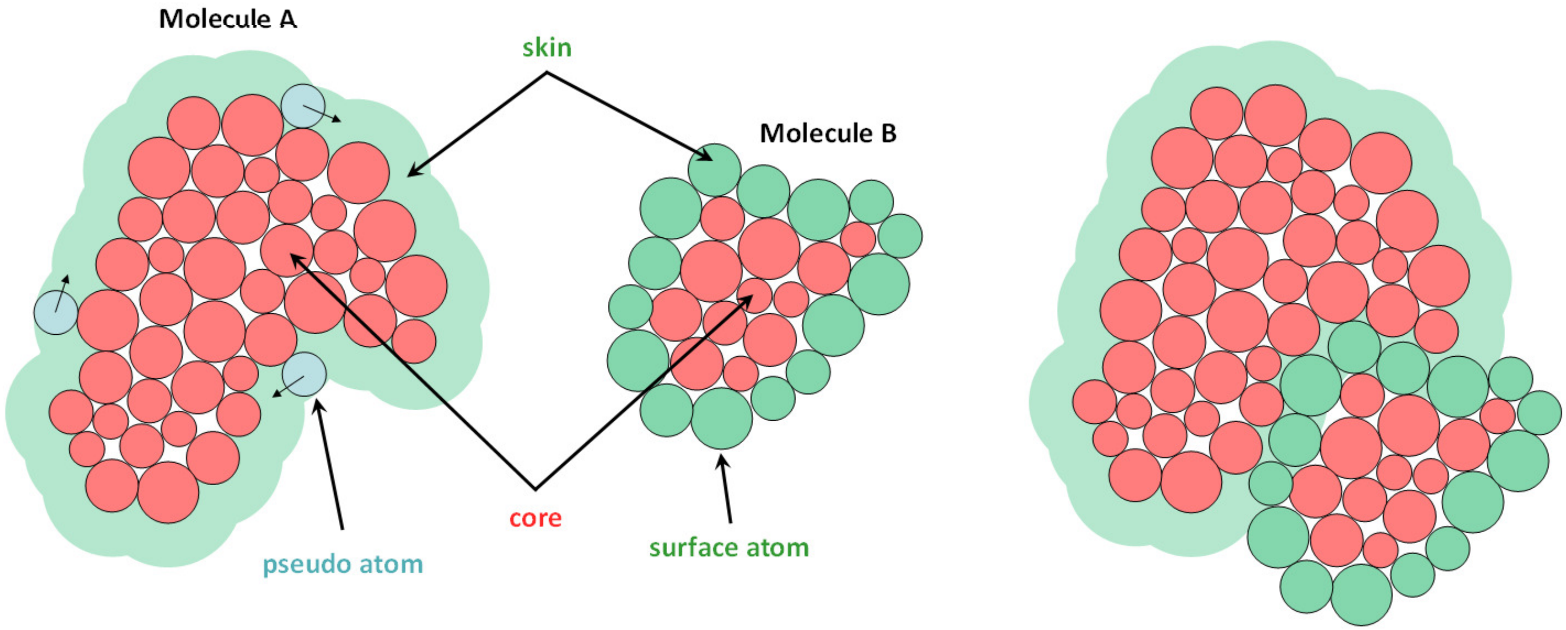
$$f_P(x) = \sum_{k=1}^{M_P} w_k \cdot g_k(x)$$

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

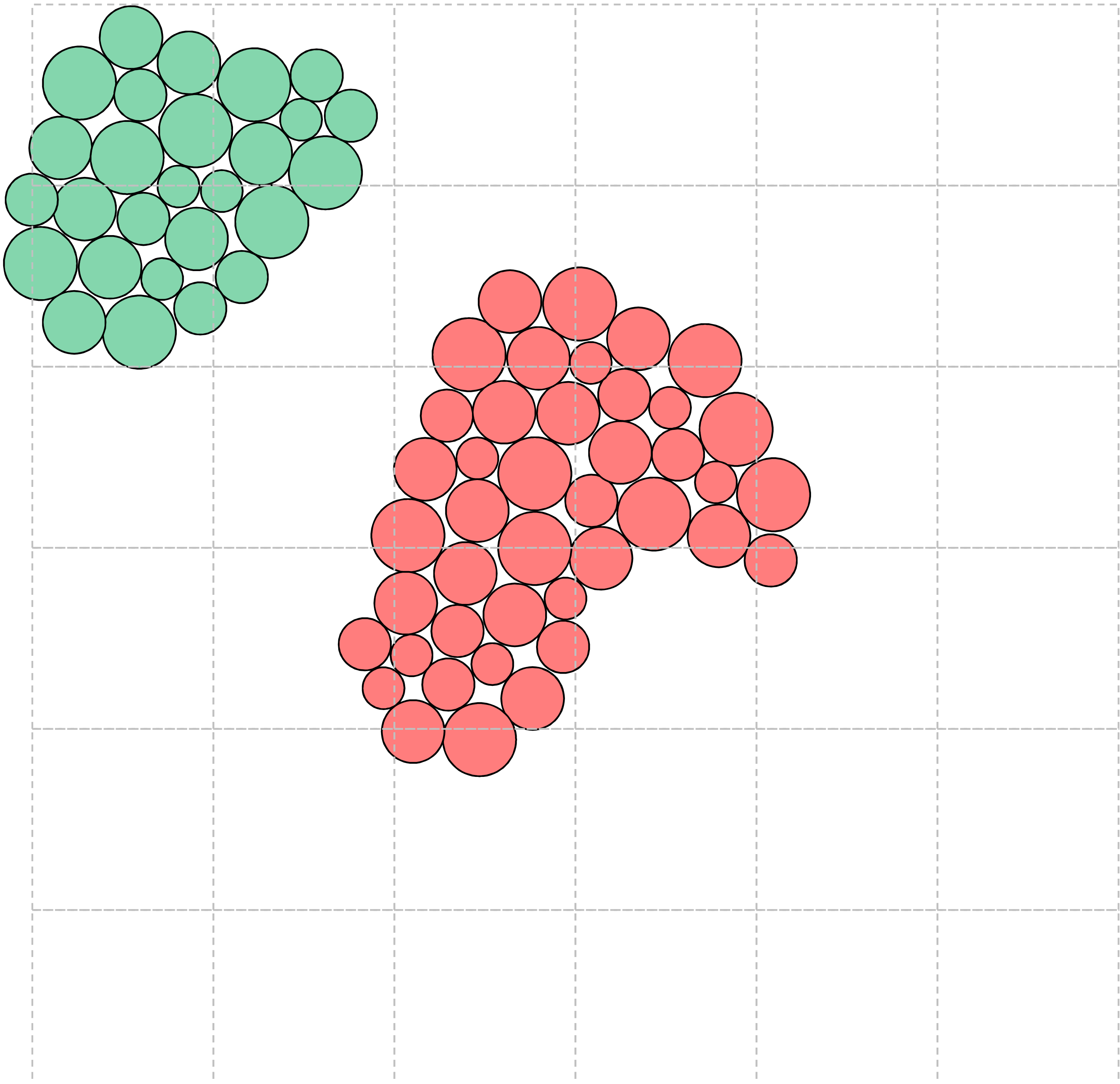
For rotation r and translation t of molecule B (i.e., $B_{t,r}$),

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

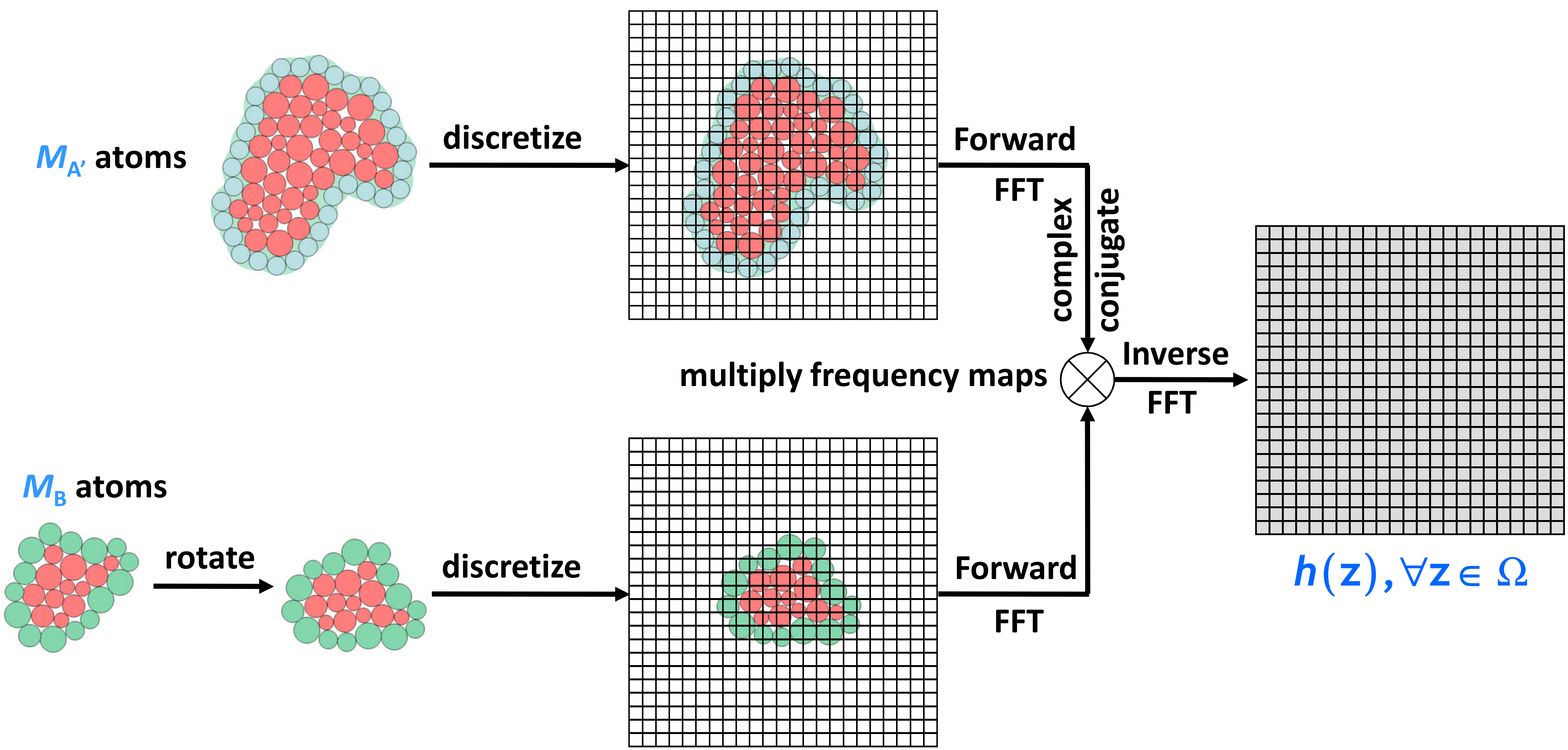
$Re\left(F_{A,B}(t,r)\right) =$ skin-skin overlap score $-$ core-core overlap score

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

Docking: Rotational & Translational Search



Translational Search using FFT



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