discrete Fourier transform

given $v(t)$ for $0 \le t \le 1$

define $\widetilde{v}_n = \int_0^1 v(t) e^{-2\pi i n t} dt$, $n = 0, \pm 1, \pm 2, \ldots$: Fourier coefficients

set $\Delta t = 1/N$, $t_j = j/N$, $j = 0 : N-1$, $v_j = v(t_j)$

then $\widetilde{v}_n \approx \sum_{j=0}^{N-1} v_j e^{-2\pi i n t_j} \Delta t = \frac{1}{N} \sum_{j=0}^{N-1} v_j e^{-2\pi i n j/N} = \frac{1}{\sqrt{N}} \widehat{v}_n$

define $\widehat{v}_n = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} v_j e^{-2\pi i n j/N}$, $n = 0 : N-1$: discrete Fourier coefficients

matrix form of DFT

$$\widehat{v}_n = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} v_j \omega^{nj} = \sum_{j=0}^{N-1} F_{nj} v_j = (Fv)_n \Rightarrow \widehat{v} = Fv$$

$\omega = e^{-2\pi i/N} \Rightarrow \omega^N = 1$

$F_{nj} = \frac{1}{\sqrt{N}} \omega^{nj}$, $j = 0 : N-1$, $n = 0 : N-1$

$v = (v_0, v_1, \ldots, v_{N-1})^T \in \mathbb{C}^N$, $\widehat{v} = (\widehat{v}_0, \widehat{v}_1, \ldots, \widehat{v}_{N-1})^T \in \mathbb{C}^N$

$$F_N = \frac{1}{\sqrt{N}} \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega & \omega^2 & \cdots & \omega^{N-1} \\ 1 & \omega^2 & \omega^4 & \cdots & \omega^{2(N-1)} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & \omega^{N-1} & \omega^{2(N-1)} & \cdots & \omega^{(N-1)^2} \end{pmatrix} , \quad F_N \in \mathbb{C}^{N \times N}$$

$$N = 2 , \ \omega = -1 , \ F_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & \omega \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$N = 4 , \ \omega = -i , \ F_4 = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega & \omega^2 & \omega^3 \\ 1 & \omega^2 & \omega^4 & \omega^6 \\ 1 & \omega^3 & \omega^6 & \omega^9 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -i & -1 & i \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \end{pmatrix}$$

<u>claim</u>

1. F is symmetric, i.e. $F^T = F$, but F is not hermitian, i.e. $F^* \neq F$.

2. F is unitary, i.e. $F^*F = I$ and $F^{-1} = F^*$.

<u>pf</u>

1. <u>ok</u>

2. $(F^*F)_{nj} = \displaystyle\sum_{k=0}^{N-1} F^*_{nk}F_{kj} = \frac{1}{N}\sum_{k=0}^{N-1} \overline{\omega}^{kn}\,\omega^{kj} = \frac{1}{N}\sum_{k=0}^{N-1} \omega^{(j-n)k}$, $\overline{\omega} = \omega^{-1}$

$$= \begin{cases} \dfrac{1}{N}\cdot\dfrac{\omega^{(j-n)N}-1}{\omega^{(j-n)}-1} & \text{if } n \neq j \\ 1 & \text{if } n = j \end{cases} = \begin{cases} 0 & \text{if } n \neq j \\ 1 & \text{if } n = j \end{cases} \quad \underline{\text{ok}}$$

recall : $\displaystyle\sum_{k=0}^{N-1} r^k = \begin{cases} \dfrac{r^N-1}{r-1} & \text{if } r \neq 1 \\ N & \text{if } r = 1 \end{cases}$

<u>note</u>

1. $\widehat{v} = Fv \Rightarrow v = F^*\widehat{v}$: inverse DFT , $v_j = \displaystyle\frac{1}{\sqrt{N}}\sum_{n=0}^{N-1}\widehat{v}_n e^{2\pi inj/N}$

2. The columns of F^* are an orthonormal basis for $\mathbb{C}^N$ (discrete Fourier basis).

<u>example</u> : $v(t) = \sin 2\pi kt$

assume $1 \leq k \leq N/2$

$$v_j = \sin 2\pi kt_j = \frac{e^{2\pi ikj/N} - e^{-2\pi ikj/N}}{2i} = \frac{e^{2\pi ikj/N} - e^{2\pi i(N-k)j/N}}{2i}$$

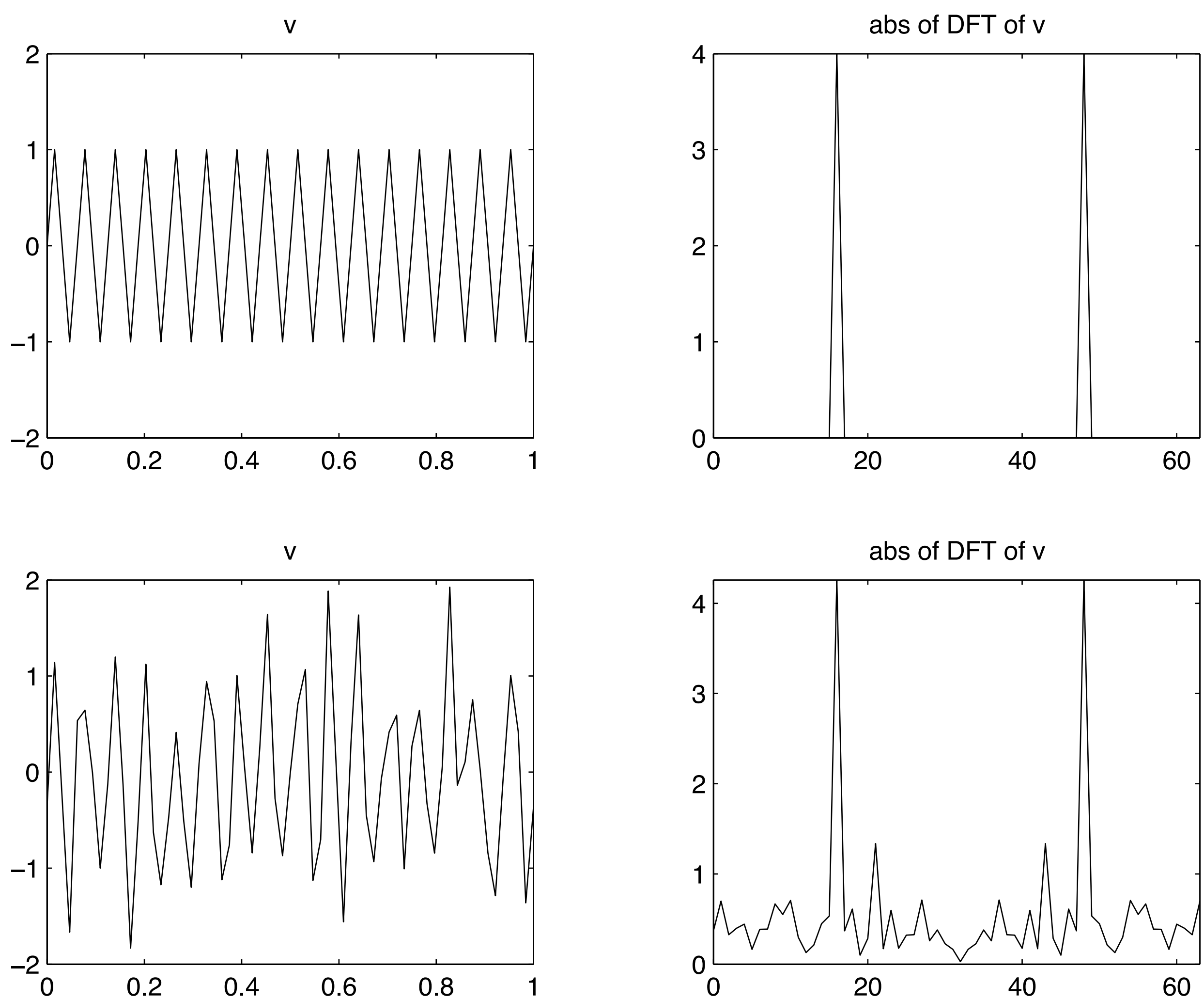
$$\Rightarrow \widehat{v}_n = \begin{cases} \sqrt{N}/2i & \text{if } n = k \\ -\sqrt{N}/2i & \text{if } n = N-k \\ 0 & \text{otherwise} \end{cases} \quad , \text{ check by direct calculation} \ldots$$

for example : $N = 64$, $k = 16$

$v_j = \sin 2\pi\cdot 16\cdot j/64 = \sin j\pi/2 \Rightarrow |\widehat{v}_{16}| = |\widehat{v}_{48}| = 4$, all other $\widehat{v}_n = 0$

question : what happens when $k = N/2$?

```
% Matlab code for demonstrating DFT
N = 64;
dt = 1/N;
t = 0:dt:1;
k=16;
frame = 1;
for icase = 1:2
  v = sin(2*pi*k*t);
  if icase==2; v = v + 0.5*randn(1,N+1); frame = 3; end
  subplot(2,2,frame); plot(t,v); axis([0 1 -2 2]); title('v');
  vhat = fft(v,N)/sqrt(N); n = 0:N-1;
  subplot(2,2,frame+1); plot(n,abs(vhat));
  axis([0 N-1 0 max(abs(vhat))]); title('abs of DFT of v');
end
```



note

Computing $\widehat{v} = Fv$ by direct matrix-vector multiplication requires $O(N^2)$ operations, but F is a structured matrix with only N distinct entries and there is a fast algorithm (FFT) that requires only $O(N \log N)$ operations.

consider $N = 8$, $\widehat{v} = F_8 v$, $\omega = e^{-2\pi i/N} = e^{-\pi i/4}$

$$\widehat{v}_n = \tfrac{1}{\sqrt{8}}\big(v_0 + v_1\omega^n + v_2\omega^{2n} + v_3\omega^{3n} + v_4\omega^{4n} + v_5\omega^{5n} + v_6\omega^{6n} + v_7\omega^{7n}\big)$$

$$= \tfrac{1}{\sqrt{8}}\Big(v_0 + v_2(\omega^2)^n + v_4(\omega^2)^{2n} + v_6(\omega^2)^{3n} + \omega^n\big(v_1 + v_3(\omega^2)^n + v_5(\omega^2)^{2n} + v_7(\omega^2)^{3n}\big)\Big)$$

$\Rightarrow$ 1 DFT of length $N \approx 2$ DFTs of length $N/2$

lemma (Danielson-Lanczos)

$$F_N = F_{2M} = \frac{1}{\sqrt{2}} B_{2M}(F_M \oplus F_M)P_{2M}$$

$$B_{2M} = \begin{pmatrix} I_M & \Omega_M \\ I_M & -\Omega_M \end{pmatrix} \ , \ \Omega_M = \mathrm{diag}\big(\underset{\substack{\uparrow \\ e^{-2\pi in/2M} = \omega^n \ , \text{ where } \omega = e^{-2\pi i/N}}}{e^{-\pi in/M}}\big) \ , \ n = 0 : M-1 \ : \ \underline{\text{butterfly}}$$

$$F_M \oplus F_M = \begin{pmatrix} F_M & 0 \\ 0 & F_M \end{pmatrix}$$

$$P_{2M} = \begin{pmatrix} P_M^e \\ P_M^o \end{pmatrix} \ , \ \left.\begin{matrix} (P_M^e)_{mn} = \delta_{2m,n} \\ (P_M^o)_{mn} = \delta_{2m+1,n} \end{matrix}\right\} \text{ for } m = 0 : M-1 \ , \ n = 0 : 2M-1$$

example : $M = 4$, $2M = 8$

$$P_8 = \begin{pmatrix} P_4^e \\ P_4^o \end{pmatrix} = \begin{pmatrix} 1&0&0&0&0&0&0&0 \\ 0&0&1&0&0&0&0&0 \\ 0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&0&1&0 \\ 0&1&0&0&0&0&0&0 \\ 0&0&0&1&0&0&0&0 \\ 0&0&0&0&0&1&0&0 \\ 0&0&0&0&0&0&0&1 \end{pmatrix} \ , \ v = \begin{pmatrix} v_0 \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \end{pmatrix} \Rightarrow P_8 v = \begin{pmatrix} v_0 \\ v_2 \\ v_4 \\ v_6 \\ v_1 \\ v_3 \\ v_5 \\ v_7 \end{pmatrix}$$

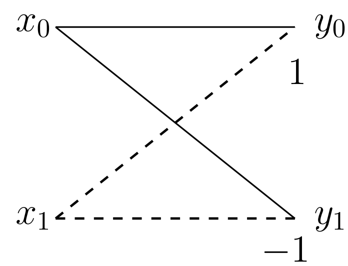
in general if $v \in \mathbb{C}^{2M}$, then $\left.\begin{matrix} (P_M^e v)_m = v_{2m} \\ (P_M^o v)_m = v_{2m+1} \end{matrix}\right\}$ for $m = 0 : M-1$

note : $Pv \to v$: shuffle $\Rightarrow$ $v \to Pv$: unshuffle

<u>why butterfly?</u>

consider $N = 2$, $\omega = e^{-2\pi i/N} = -1$

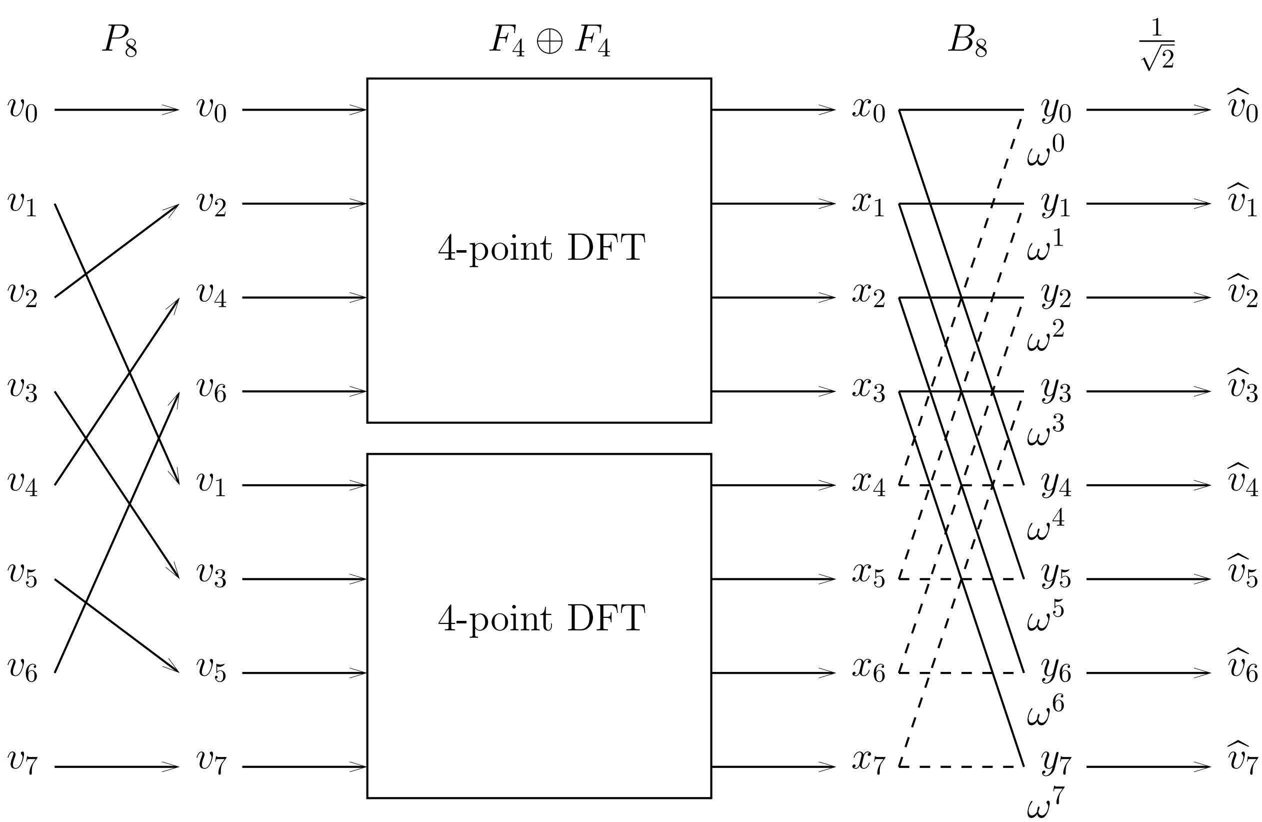
$$B_2 = \begin{pmatrix} 1 & \omega^0 \\ 1 & -\omega^0 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \; B_2 \begin{pmatrix} x_0 \\ x_1 \end{pmatrix} = \begin{pmatrix} x_0 + x_1 \\ x_0 - x_1 \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \end{pmatrix}$$



$$N = 8\,,\; B_8 = \left(\begin{array}{cccc|cccc} 1 & 0 & 0 & 0 & \omega^0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & \omega^1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & \omega^2 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & \omega^3 \\ \hline 1 & 0 & 0 & 0 & -\omega^0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -\omega^1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -\omega^2 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\omega^3 \end{array}\right),\; \omega = e^{-2\pi i/8} = e^{-\pi i/4}$$

note : $(-\omega^0, -\omega^1, -\omega^2, -\omega^3) = (\omega^4, \omega^5, \omega^6, \omega^7)$

8-point DFT : $F_8 v \;=\; \frac{1}{\sqrt{2}}\, B_8\,(F_4 \oplus F_4)\, P_8 v \;=\; \widehat{v}$



<u>pf</u>

$$\big(F_{2M}v\big)_n = \frac{1}{\sqrt{2M}} \sum_{j=0}^{2M-1} v_j e^{-2\pi i n j/2M}$$

$$= \frac{1}{\sqrt{2M}} \left(\sum_{j=0}^{M-1} v_{2j} e^{-2\pi i n(2j)/2M} + \sum_{j=0}^{M-1} v_{2j+1} e^{-2\pi i n(2j+1)/2M} \right)$$

$$= \frac{1}{\sqrt{2M}} \left(\sum_{j=0}^{M-1} (P_M^e v)_j e^{-2\pi i n j/M} + e^{-\pi i n/M} \sum_{j=0}^{M-1} (P_M^o v)_j e^{-2\pi i n j/M} \right)$$

Each term involves an M-point DFT.

$$\frac{1}{\sqrt{2}} B_{2M}(F_M \oplus F_M) P_{2M}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} I_M & \Omega_M \\ I_M & -\Omega_M \end{pmatrix} \begin{pmatrix} F_M & 0 \\ 0 & F_M \end{pmatrix} \begin{pmatrix} P_M^e \\ P_M^o \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} F_M & \Omega_M F_M \\ F_M & -\Omega_M F_M \end{pmatrix} \begin{pmatrix} P_M^e \\ P_M^o \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} F_M P_M^e + \Omega_M F_M P_M^o \\ F_M P_M^e - \Omega_M F_M P_M^o \end{pmatrix}$$

<u>case 1</u> : $n = 0 : M-1$

$$\big(F_{2M}v\big)_n = \frac{1}{\sqrt{2}} \big((F_M P_M^e v)_n + (\Omega_M F_M P_M^o v)_n \big)$$

<u>case 2</u> : $n = M : 2M-1$

for an M-point DFT , we need to replace n by $n-M$

$e^{-2\pi i n j/M} = e^{-2\pi i (n-M) j/M}$, $e^{-\pi i n/M} = -e^{-\pi i (n-M)/M}$

$$\big(F_{2M}v\big)_n = \frac{1}{\sqrt{2}} \big((F_M P_M^e v)_{n-M} - (\Omega_M F_M P_M^o v)_{n-M} \big) \quad \underline{\text{ok}}$$

thm (FFT)

Let $N = 2^q$, $q \geq 1$.

Then $F_N = \dfrac{1}{\sqrt{N}} A_0^N A_1^N \cdots A_{q-1}^N P^N$, where P^N is a certain permutation matrix,

$A_0^N = B_N$: 1 term,

$A_1^N = B_{N/2} \oplus B_{N/2}$: 2 terms,

$A_2^N = B_{N/4} \oplus B_{N/4} \oplus B_{N/4} \oplus B_{N/4}$: 4 terms,

$\cdots$

$A_{q-1}^N = B_{N/2^{q-1}} \oplus \cdots \oplus B_{N/2^{q-1}} = B_2 \oplus \cdots \oplus B_2$: $2^{q-1} = N/2$ terms,

and superscript N is the matrix dimension, not an N-fold product.

pf : induction on q

If $q = 1$, then $N = 2$, $A_0^2 = B_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, and let $P^2 = I_2$.

Then $F_2 = \dfrac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \dfrac{1}{\sqrt{2}} A_0^2 P^2$ as required.

Assume true for $M = 2^{q-1}$, must show true for $N = 2^q = 2M$.

2 preliminary facts

1. $A_k^N = B_{N/2^k} \oplus \cdots \oplus B_{N/2^k}$: 2^k terms

$= B_{M/2^{k-1}} \oplus \cdots \oplus B_{M/2^{k-1}}$: $2 \cdot 2^{k-1}$ terms

$= A_{k-1}^M \oplus A_{k-1}^M$

2. $(A \oplus B)(C \oplus D) = AC \oplus BD$: $\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & D \end{pmatrix} = \begin{pmatrix} AC & 0 \\ 0 & BD \end{pmatrix}$

$$F_N = \frac{1}{\sqrt{2}} B_N (F_M \oplus F_M) P_N$$

$$= \frac{1}{\sqrt{2}} A_0^N \left(\frac{1}{\sqrt{M}} A_0^M A_1^M \cdots A_{q-2}^M P^M \oplus \frac{1}{\sqrt{M}} A_0^M A_1^M \cdots A_{q-2}^M P^M \right) P_N$$

$$= \frac{1}{\sqrt{2M}} A_0^N (A_0^M \oplus A_0^M)(A_1^M \oplus A_1^M) \cdots (A_{q-2}^M \oplus A_{q-2}^M)(P^M \oplus P^M) P_N$$

$$= \frac{1}{\sqrt{N}} A_0^N A_1^N A_2^N \cdots A_{q-1}^N P^N \text{ , where } P^N = (P^M \oplus P^M) P_N \quad \underline{\text{ok}}$$

<u>operation count</u> for computing $F_N v = \dfrac{1}{\sqrt{N}} A_0^N A_1^N \cdots A_{q-1}^N P^N v$

applying P^N : 0 flops (more soon)

A_k^N has 2 nonzero entries in each row : $2N$ flops

multiplication by $\dfrac{1}{\sqrt{N}}$: N flops

total : $2N \cdot q + N$ flops , $q = \log_2 N \Rightarrow O(N \log_2 N)$ flops

<u>interpretation of P^N</u>

Let $N = 2^q$. Then any n st $0 \le n \le N-1$ can be written as

$n = b_0 + b_1 \cdot 2 + b_2 \cdot 4 + \cdots + b_{q-1} \cdot 2^{q-1}$, where $b_j \in \{0, 1\}$.

$n = (b_{q-1}\, b_{q-2} \cdots b_1\, b_0)_2$

$n' = (b_{q-2} \cdots b_1\, b_0\, b_{q-1})_2$: N-point periodic shift

$n'' = (b_0\, b_1 \cdots b_{q-2}\, b_{q-1})_2$: N-point bit reversal

<u>example</u> : $q = 3$, $N = 8$

n	n'	n''
000	000	000
001	010	100
010	100	010
011	110	110
100	001	001
101	011	101
110	101	011
111	111	111

n	n'	n''
0	0	0
1	2	4
2	4	2
3	6	6
4	1	1
5	3	5
6	5	3
7	7	7

<u>claim</u> : $(P_N v)_n = v_{n'}$, $(P^N v)_n = v_{n''}$

<u>pf</u> : $N = 2^q = 2M$, $0 \le n \le N-1$

define $m = (b_{q-2} \cdots b_1\, b_0)_2$, so $0 \le m \le M-1$

then $n = b_{q-1} \cdot 2^{q-1} + m$, $n' = 2m + b_{q-1}$

1. $(P_N v)_n = \begin{cases} (P_M^e v)_m & \text{if } b_{q-1} = 0 \\ (P_M^o v)_m & \text{if } b_{q-1} = 1 \end{cases} = \begin{cases} v_{2m} & \text{if } b_{q-1} = 0 \\ v_{2m+1} & \text{if } b_{q-1} = 1 \end{cases} = v_{2m+b_{q-1}} = v_{n'}$

2. induction on q

$q = 1 \Rightarrow N = 2$, $P^2 = I_2$, $0 \le n \le 1$, $n = (b_0)_2 = n''$

now let $M = N/2$ and assume P^M does M-point bit reversal

must show $P^N = (P^M \oplus P^M)P_N$ does N-point bit reversal

$n'' = (b_0\, b_1\, \cdots\, b_{q-2}\, b_{q-1})_2 \;=\; 2m'' + b_{q-1}$

$$P^N = (P^M \oplus P^M)\begin{pmatrix} P_M^e \\ P_M^o \end{pmatrix} = \begin{pmatrix} P^M P_M^e \\ P^M P_M^o \end{pmatrix}$$

$$(P^N v)_n \;=\; \begin{cases} (P^M P_M^e v)_m & \text{if } \; b_{q-1} = 0 \\ (P^M P_M^o v)_m & \text{if } \; b_{q-1} = 1 \end{cases} \;=\; \begin{cases} (P_M^e v)_{m''} & \text{if } \; b_{q-1} = 0 \\ (P_M^o v)_{m''} & \text{if } \; b_{q-1} = 1 \end{cases}$$

$$= \begin{cases} v_{2m''} & \text{if } \; b_{q-1} = 0 \\ v_{2m''+1} & \text{if } \; b_{q-1} = 1 \end{cases} \;=\; v_{2m''+b_{q-1}} \;=\; v_{n''} \qquad \underline{\text{ok}}$$

<u>note</u>

1. FFT is based on divide-and-conquer, recursion, sparse factorization

2. $O(N \log N)$ flops, but this neglects memory access/communication

3. inverse FFT : $F_N^{-1} = F_N^* = \overline{F_N} = \dfrac{1}{\sqrt{N}}\, \overline{A_0^N}\;\, \overline{A_1^N} \cdots \overline{A_{q-1}^N}\; P^N$

4. variants

DST : $\widehat{v}_n = \sqrt{\dfrac{2}{N}}\, \displaystyle\sum_{j=1}^{N-1} v_j \sin\frac{\pi n j}{N}$, $n = 1 : N-1$

5. multi-dimensional versions

6. FFTW : code adapts to the machine it's running on, auto-tuning

<u>application</u> : trigonometric interpolation

Let $v(x)$ be given for $0 \le x \le 1$ and assume $v(0) = v(1)$.

$$v(x) = \sum_{n=-\infty}^{\infty} \widetilde{v}_n \, e^{2\pi i n x} \ , \ \widetilde{v}_n = \int_0^1 v(x) e^{-2\pi i n x} dx \ : \ \text{Fourier series}$$

set $v_j = v(x_j)$, $x_j = j/N$, $j = 0 : N-1$: uniform mesh

$$v_j = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \widehat{v}_n e^{2\pi i n x_j} \ , \ \widehat{v}_n = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} v_j e^{-2\pi i n x_j} \ , \ \text{pf} : \ v = F^* F v = F^* \widehat{v}$$

$$\text{set} \ \ I_1(x) = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \widehat{v}_n e^{2\pi i n x} \ : \ \text{trigonometric polynomial}$$

then $I_1(x) \approx v(x)$, two sources of error : finite N , $\dfrac{1}{\sqrt{N}} \widehat{v}_n \neq \widetilde{v}_n$

Note that $I_1(x_j) = v_j$ for $j = 0 : N-1$, i.e. $I_1(x)$ <u>interpolates</u> $v(x)$ at $x = x_j$. However, $I_1(x)$ is a poor approximation to $v(x)$ in between the mesh points; consider instead a balanced set of wavenumbers.

$$\text{set} \ \ I_2(x) = \frac{1}{\sqrt{N}} \sum_{n=-N/2}^{N/2-1} \widehat{v}_{n \bmod N} \, e^{2\pi i n x} \ , \ n \bmod N = \begin{cases} n & \text{if} \ \ n = 0 : N/2-1 \\ n+N & \text{if} \ \ n = -N/2 : -1 \end{cases}$$

1. e.g. $7 \bmod 16 = 7$, $-7 \bmod 16 = 9$

2. a similar formula is used if N is odd

$$\begin{aligned}
I_2(x_j) &= \frac{1}{\sqrt{N}} \sum_{n=-N/2}^{N/2-1} \widehat{v}_{n \bmod N} \, e^{2\pi i n x_j} \\
&= \frac{1}{\sqrt{N}} \left(\sum_{n=0}^{N/2-1} \widehat{v}_n \, e^{2\pi i n j/N} + \sum_{n=-N/2}^{-1} \widehat{v}_{n+N} \, e^{2\pi i n j/N} \right) \\
&= \frac{1}{\sqrt{N}} \left(\sum_{n=0}^{N/2-1} \widehat{v}_n \, e^{2\pi i n j/N} + \sum_{n=N/2}^{N-1} \widehat{v}_n \, e^{2\pi i (n-N) j/N} \right) \\
&= \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \widehat{v}_n \, e^{2\pi i n j/N} = v_j
\end{aligned}$$

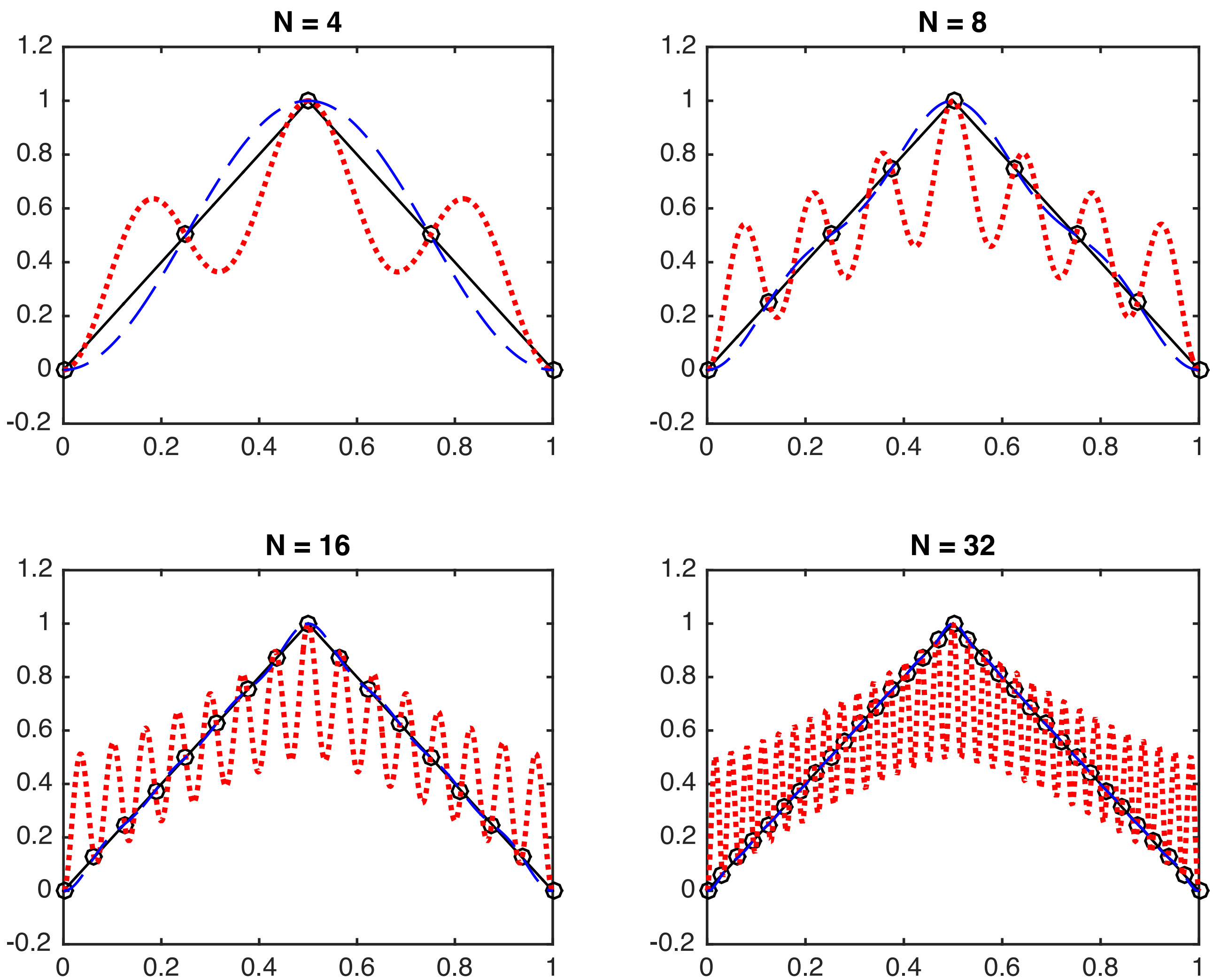
Hence $I_2(x)$ also interpolates $v(x)$ at $x = x_j$, but it gives a better approximation in between the mesh points.

trigonometric interpolation

$$v(x) = 1 - 2\left|x - \tfrac{1}{2}\right|$$

$$I_1(x) = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \widehat{v}_n e^{2\pi i n x} \;:\; \text{unbalanced}$$

$$I_2(x) = \frac{1}{\sqrt{N}} \sum_{n=-N/2}^{N/2-1} \widehat{v}_{n \bmod N}\, e^{2\pi i n x} \;:\; \text{balanced}$$



1. The balanced interpolant converges uniformly to the given function as $N \to \infty$, i.e. $\lim_{N\to\infty} \max_{0\le x\le 1} |v(x) - I_2(x)| = 0$.

2. The unbalanced interpolant does not converge uniformly to the given function.

<u>application</u> : BVP

given $f(x)$ for $0 \le x \le 1$ and $\sigma > 0$

find $\phi(x)$ st $-\phi'' + \sigma^2\phi = f$, $\phi(0) = \phi(1)$, $\phi'(0) = \phi'(1)$: PBC

We will consider 3 solution methods: finite-differences, pseudospectral, Green's function.

<u>finite-difference scheme</u>

set $h = 1/N$, $x_j = jh = j/N$ for $j = 0 : N-1$, $\phi_j = \phi(x_j)$, $f_j = f(x_j)$

$\phi_j'' = D_+D_-\phi_j + O(h^2)$, where $D_+D_-\phi_j = \dfrac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{h^2}$

u_j : numerical solution , $u_j \approx \phi_j$

$$-D_+D_-u_j + \sigma^2 u_j = f_j \ \Rightarrow\ \frac{-u_{j+1} + (2+\sigma^2h^2)u_j - u_{j-1}}{h^2} = f_j$$

$$j = 0 \ \Rightarrow\ \frac{-u_1 + (2+\sigma^2h^2)u_0 - u_{-1}}{h^2} = f_0 \,,\ u_{-1} = \,?$$

$$j = N-1 \ \Rightarrow\ \frac{-u_N + (2+\sigma^2h^2)u_{N-1} - u_{N-2}}{h^2} = f_{N-1} \,,\ u_N = \,?$$

PBC $\Rightarrow$ $\phi(x+1) = \phi(x)$, so we set $u_{-1} = u_{N-1}$, $u_N = u_0$

$$\frac{1}{h^2}\begin{pmatrix} 2+\sigma^2h^2 & -1 & & & & -1 \\ -1 & 2+\sigma^2h^2 & -1 & & & \\ \ddots & \ddots & \ddots & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2+\sigma^2h^2 & -1 \\ -1 & & & & -1 & 2+\sigma^2h^2 \end{pmatrix}\begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ \vdots \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ \vdots \\ \vdots \\ f_{N-2} \\ f_{N-1} \end{pmatrix}$$

$Au = f$, A : symmetric, positive definite, almost tridiagonal, ...

solution methods : Cholesky, SOR, conjugate gradient, multigrid, FFT, ...

claim : The e-vectors of A are the columns of F_N^*.

pf : Let q be the nth column of F_N^* for some $n = 0 : N-1$.

$$q = \frac{1}{\sqrt{N}}(1\,,\,\omega^{-n},\,\omega^{-2n},\,\ldots\,,\,\omega^{-(N-1)n})^T\,,\;\omega = e^{-2\pi i/N} = e^{-2\pi i h}$$

$Aq = \lambda q \;\Leftrightarrow\; (Aq)_j = \lambda q_j$ for $j = 0 : N-1$, assume $N \geq 3$

$$(Aq)_j \;=\; \frac{-q_{j+1} + (2+\sigma^2h^2)q_j - q_{j-1}}{h^2}\;\;,\text{ set } q_{-1} = q_{N-1}\,,\; q_N = q_0$$

$$\Rightarrow\; \frac{1}{\sqrt{N}}\frac{-\omega^{-(j+1)n} + (2+\sigma^2h^2)\omega^{-jn} - \omega^{-(j-1)n}}{h^2} \;=\; \lambda\frac{1}{\sqrt{N}}\,\omega^{-jn}$$

$$\Rightarrow\; \lambda \;=\; \frac{-\omega^{-n} + (2+\sigma^2h^2) - \omega^{n}}{h^2} \;=\; \sigma^2 + \frac{2 - (e^{2\pi inh} + e^{-2\pi inh})}{h^2}$$

$$=\; \sigma^2 + \frac{2(1-\cos 2\pi nh)}{h^2} \;=\; \sigma^2 + \frac{4\sin^2\!\pi nh}{h^2} \qquad \underline{\text{ok}}$$

note : $AF_N^* = F_N^*D$, $D = \text{diag}(\lambda_0,\ldots,\lambda_{N-1})$, $\lambda_n = \sigma^2 + \dfrac{4\sin^2\!\pi nh}{h^2}$

$\Rightarrow A = F_N^*DF_N$: spectral factorization

$Au = f \;\Rightarrow\; u = A^{-1}f = F_N^*D^{-1}F_Nf$: $O(N\log N)$ flops

Next we show that this is a general fact.

def : given $(c_0,\ldots,c_{N-1})^T$, define $C = (C_{nj}) = c_{(n-j)\bmod N}$: circulant matrix

example : $N = 6$

$$\begin{pmatrix} c_0 & c_5 & c_4 & c_3 & c_2 & c_1 \\ c_1 & c_0 & c_5 & c_4 & c_3 & c_2 \\ c_2 & c_1 & c_0 & c_5 & c_4 & c_3 \\ c_3 & c_2 & c_1 & c_0 & c_5 & c_4 \\ c_4 & c_3 & c_2 & c_1 & c_0 & c_5 \\ c_5 & c_4 & c_3 & c_2 & c_1 & c_0 \end{pmatrix}$$

1. A circulant matrix has constant diagonals, and each column is a periodic shift of the previous column.

2. The finite-difference matrix is circulant.

$$c_0 = \frac{2+\sigma^2h^2}{h^2}\,,\; c_1 = -\frac{1}{h^2}\,,\; c_2 = 0\,,\;\ldots\,,\; c_{N-2} = 0\,,\; c_{N-1} = -\frac{1}{h^2}$$

<u>def</u>

$c * v \,=\, Cv \,:\,$ <u>convolution</u>

$$(c*v)_n \,=\, (Cv)_n \,=\sum_{j=0}^{N-1} C_{nj} v_j \,=\sum_{j=0}^{N-1} c_{(n-j)\mathrm{mod}N} v_j$$

$$= c_{n\mathrm{mod}N} v_0 \,+\, c_{(n-1)\mathrm{mod}N} v_1 \,+\, \cdots \,+\, c_{(n-(N-1))\mathrm{mod}N} v_{N-1}$$

<u>example</u> : $N = 6\,,\ n = 3 \;\Rightarrow\; (c*v)_3 \,=\, c_3v_0 + c_2v_1 + c_1v_2 + c_0v_3 + c_5v_4 + c_4v_5$

<u>claim</u>

1. $(c*v)\widehat{\ } = \sqrt{N}\,\widehat{c}\,\widehat{v}$: component-wise product

2. $\langle c\,,v\rangle = \langle \widehat{c}\,,\widehat{v}\rangle$, where $\langle c\,,v\rangle = \sum_{j=0}^{N-1} c_j \overline{v_j}$: inner product

3. $C = F_N^* D F_N$, where $D = \mathrm{diag}\big(\sqrt{N}\,\widehat{c}_n\big)$

<u>pf</u>

1. $(c*v)\widehat{_n} = (F_N(c*v))_n \,= \dfrac{1}{\sqrt{N}}\sum_{j=0}^{N-1} \omega^{nj}(c*v)_j$, $\omega = e^{-2\pi i/N}$, $\omega^N = 1$

$$= \frac{1}{\sqrt{N}}\sum_{j=0}^{N-1}\omega^{nj}\sum_{k=0}^{N-1} c_{(j-k)\mathrm{mod}N} v_k$$

$$= \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}\ \sum_{j=0}^{N-1}\omega^{n(j-k)} c_{(j-k)\mathrm{mod}N}\cdot\omega^{nk} v_k \quad , \ \text{set } \ell = j-k$$

$$= \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}\ \sum_{\ell=-k}^{N-1-k}\omega^{n\ell} c_{\ell\mathrm{mod}N}\cdot\omega^{nk} v_k \,=\, \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}\ \sum_{\ell=0}^{N-1}\omega^{n\ell} c_\ell\cdot\omega^{nk} v_k$$

$$= \frac{1}{\sqrt{N}}\sum_{\ell=0}^{N-1}\omega^{n\ell} c_\ell\cdot\sum_{k=0}^{N-1}\omega^{nk} v_k = \sqrt{N}\,\widehat{c}_n\widehat{v}_n$$

2. $\langle \widehat{c}\,,\widehat{v}\rangle = \langle F_N c\,, F_N v\rangle = \langle c\,, F_N^* F_N v\rangle = \langle c\,,v\rangle$, check . . .

3. Let p and q be the mth and nth columns of F_N^*.

$F_N^* e_m = p\ ,\ F_N^* e_n = q \;\Rightarrow\; e_m = F_N p = \widehat{p}\ ,\ e_n = F_N q = \widehat{q}$

$\langle Cp\,,q\rangle = \langle c*p\,,q\rangle = \langle (c*p)\widehat{\ },\widehat{q}\,\rangle = \langle \sqrt{N}\,\widehat{c}\,\widehat{p}\,,\widehat{q}\,\rangle = \langle \sqrt{N}\,\widehat{c}\,e_m\,,\widehat{q}\,\rangle$

$$= \langle \sqrt{N}\,\widehat{c}_m\,e_m\,,\widehat{q}\,\rangle = \langle De_m\,,\widehat{q}\,\rangle = \langle DF_N p\,, F_N q\rangle = \langle F_N^* D F_N p\,,q\rangle \qquad \underline{\text{ok}}$$

note : The general expression for D agrees with the result derived for the e-values of the finite-difference matrix A. (hw2) pseudospectral method

given u_j , $j = 0 : N-1$

recall : $I_2(x) = \dfrac{1}{\sqrt{N}} \displaystyle\sum_{n=-N/2}^{N/2-1} \widehat{u}_{n\mathrm{mod}N}\, e^{2\pi i n x}$, $I_2(x_j) = u_j$, $x_j = jh$, $1/N$

$$\text{set } u'_j = I'_2(x_j) = \frac{1}{\sqrt{N}} \sum_{n=-N/2}^{N/2-1} \widehat{u}_{n\mathrm{mod}N}\, 2\pi i n\, e^{2\pi i n x_j}$$

$$= \frac{1}{\sqrt{N}} \left(\sum_{n=0}^{N/2-1} \widehat{u}_n\, 2\pi i n\, e^{2\pi i n j/N} + \sum_{n=-N/2}^{-1} \widehat{u}_{n+N}\, 2\pi i n\, e^{2\pi i n j/N} \right)$$

$$\downarrow$$

$$\sum_{n=N/2}^{N-1} \widehat{u}_n\, 2\pi i (n-N) e^{2\pi i (n-N) j/N}$$

$$= \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \widehat{u}_n d_n e^{2\pi i n j/N} \ , \ d_n = \begin{cases} 2\pi i n & \text{if } n = 0 : N/2-1 \\ 2\pi i (n-N) & \text{if } n = N/2 : N-1 \end{cases}$$

$\Rightarrow\ u' = F_N^* D F_N u$, $D = \mathrm{diag}(d_n)$

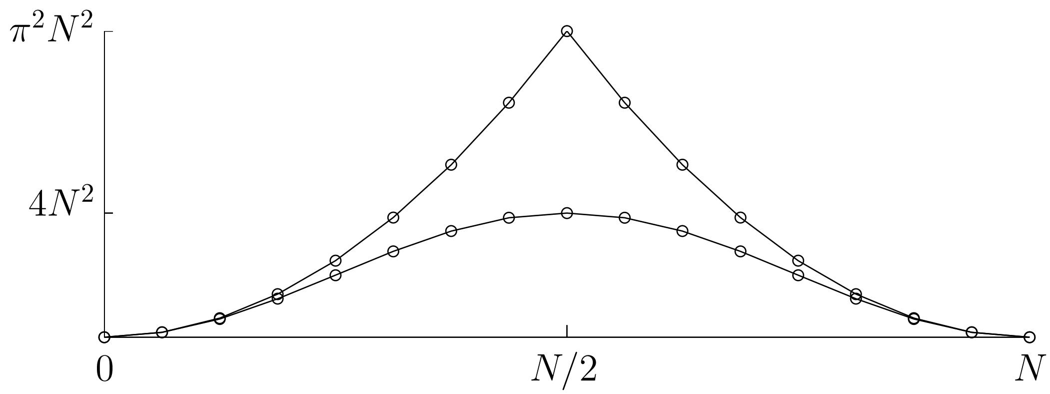
$-\phi'' + \sigma^2 \phi = f \ \rightarrow\ -F_N^* D^2 F_N u + \sigma^2 u = f$

$\Rightarrow\ F_N^*(-D^2 + \sigma^2 I) F_N u = f \ \Rightarrow\ u = F_N^*(-D^2+\sigma^2 I)^{-1} F_N f$: $O(N \log N)$ flops

1. PBC are satisfied because $I_2(x)$ is periodic.

2. The pseudospectral scheme resembles the finite-difference/FFT scheme, but the diagonal matrix representing $-\phi''$ is different.

$$-d_{n,fd}^2 = \frac{4 \sin^2 \pi n h}{h^2} \ , \ -d_{n,ps}^2 = \begin{cases} 4\pi^2 n^2 & \text{if } n = 0 : N/2-1 \\ 4\pi^2 (n-N)^2 & \text{if } n = N/2 : N-1 \end{cases}$$



<u>Green's function</u>

$-\phi'' + \sigma^2\phi = f \ , \ \phi(0) = \phi(1) \ , \ \phi'(0) = \phi'(1)$

$$g(x,y) = \frac{\cosh\sigma(|x-y| - \frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} \ , \ 0 \le x \, , \, y \le 1$$

<u>claim</u>

1. $-g_{xx}(x,y) + \sigma^2 g(x,y) = 0$ for $x \ne y$

2. $g(x,x^-) = g(x,x^+) \ , \ g_x(x,x^-) - g_x(x,x^+) = -1$

note : properties 1 and 2 $\Leftrightarrow -g_{xx}(x,y) + \sigma^2 g(x,y) = \delta(x-y)$

3. $g(0,y) = g(1,y) \ , \ g_x(0,y) = g_x(1,y)$

4. $\phi(x) = \displaystyle\int_0^1 g(x,y) f(y)\, dy$

<u>pf</u>

$$g(x,y) = \begin{cases} \dfrac{\cosh\sigma(x-y-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} & \text{if } \ 0 \le y \le x \le 1 \\[2ex] \dfrac{\cosh\sigma(y-x-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} & \text{if } \ 0 \le x \le y \le 1 \end{cases}$$

$$g_x(x,y) = \begin{cases} \dfrac{\sigma\sinh\sigma(x-y-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} & \text{if } \ 0 \le y \le x \le 1 \\[2ex] \dfrac{-\sigma\sinh\sigma(y-x-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} & \text{if } \ 0 \le x \le y \le 1 \end{cases}$$

1. <u>ok</u>

2. $g(x,x^-) = \dfrac{\cosh(-\frac{1}{2}\sigma)}{2\sigma\sinh\frac{1}{2}\sigma} = g(x,x^+)$

$$g_x(x,x^-) - g_x(x,x^+) = \frac{\sigma\sinh\sigma(-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} - \frac{-\sigma\sinh\sigma(-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} = -\frac{1}{2} - \frac{1}{2} = -1 \qquad \underline{\text{ok}}$$

3. $g(0,y) = \dfrac{\cosh\sigma(y-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} = \dfrac{\cosh\sigma(\frac{1}{2}-y)}{2\sigma\sinh\frac{1}{2}\sigma} = g(1,x)$

$$g_x(0,y) = \frac{-\sigma\sinh\sigma(y-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} = \frac{\sigma\sinh\sigma(\frac{1}{2}-y)}{2\sigma\sinh\frac{1}{2}\sigma} = g_x(1,y) \qquad \underline{\text{ok}}$$

4. define $\phi(x) = \displaystyle\int_0^1 g(x,y)f(y)\,dy$

need to show that $\phi(x)$ satisfies differential equation and PBC

$$\phi(0) = \int_0^1 g(0,y)f(y)\,dy = \int_0^1 g(1,y)f(y)\,dy = \phi(1)$$

$$\phi(x) = \int_0^x g(x,y)f(y)\,dy \,+ \int_x^1 g(x,y)f(y)\,dy$$

$$\phi'(x) = \int_0^x g_x(x,y)f(y)\,dy \,+ \int_x^1 g_x(x,y)f(y)\,dy \,+\, \cancelto{0}{(g(x,x^-) - g(x,x^+))}f(x)$$

$$\phi'(0) = \int_0^1 g_x(0,y)f(y)\,dy = \int_0^1 g_x(1,y)f(y)\,dy = \phi'(1)$$

$$\phi''(x) = \int_0^x g_{xx}(x,y)f(y)\,dy \,+ \int_x^1 g_{xx}(x,y)f(y)\,dy + \cancelto{-1}{(g_x(x,x^-) - g_x(x,x^+))}f(x)$$

$$\phi''(x) = \int_0^x \sigma^2 g(x,y)f(y)\,dy \,+ \int_x^1 \sigma^2 g(x,y)f(y)\,dy - f(x)$$

$$= \sigma^2 \int_0^1 g(x,y)f(y)\,dy - f(x) = \sigma^2\phi(x) - f(x) \qquad \underline{\text{ok}}$$

<u>discretization</u>

$$\phi(x) = \int_0^1 g(x,y)f(y)\,dy \ , \ g(x,y) = \frac{\cosh\sigma(|x-y| - \frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma}$$

$$u_j = \sum_{k=0}^{N-1} g(x_j,x_k)f_k h \ , \ x_j = jh \, , \, h = 1/N \, , \, j = 0 : N-1 \ : \ \text{Riemann sum}$$

$u = Gf$, $G_{jk} = g(x_j,x_k)h$: $O(N^2)$ ops

<u>note</u>

$g(x,y) \neq 0$, $g(x,y) = g(y,x)$, $g(x,y) = g(|x-y|,0)$

$\Rightarrow$ G : dense , symmetric , constant on diagonals claim : G is a circulant matrix

example : $N = 4$

$$G = \begin{pmatrix} g(x_0,x_0) & g(x_0,x_1) & g(x_0,x_2) & g(x_0,x_3) \\ g(x_1,x_0) & g(x_1,x_1) & g(x_1,x_2) & g(x_1,x_3) \\ g(x_2,x_0) & g(x_2,x_1) & g(x_2,x_2) & g(x_2,x_3) \\ g(x_3,x_0) & g(x_3,x_1) & g(x_3,x_2) & g(x_3,x_3) \end{pmatrix} h$$

$$= \begin{pmatrix} g(x_0,0) & g(x_1,0) & g(x_2,0) & g(x_3,0) \\ g(x_1,0) & g(x_0,0) & g(x_1,0) & g(x_2,0) \\ g(x_2,0) & g(x_1,0) & g(x_0,0) & g(x_1,0) \\ g(x_3,0) & g(x_2,0) & g(x_1,0) & g(x_0,0) \end{pmatrix} h$$

$$= \begin{pmatrix} c_0 & c_1 & c_2 & c_3 \\ c_1 & c_0 & c_1 & c_2 \\ c_2 & c_1 & c_0 & c_1 \\ c_3 & c_2 & c_1 & c_0 \end{pmatrix} = \begin{pmatrix} c_0 & c_1 & c_2 & c_1 \\ c_1 & c_0 & c_1 & c_2 \\ c_2 & c_1 & c_0 & c_1 \\ c_1 & c_2 & c_1 & c_0 \end{pmatrix} \ : \ \underline{\text{ok}}$$

$$c_3 = g(x_3,0)h = g(0,x_3)h = g(1,x_3)h = g(1-x_3,0)h = g(x_1,0)h = c_1$$

<u>pf</u> : $0 \le x\,,\, y \le 1 \Rightarrow -1 \le x - y \le 1$

$$\text{then } g(x,y) = \begin{cases} g(x-y,0) & \text{if } \quad 0 \le x-y \le 1 \\ g(x-y+1,0) & \text{if } -1 \le x-y \le 0 \end{cases}$$

the case $0 \le x - y \le 1$ is clear , check the case $-1 \le x - y \le 0$

$$g(x-y+1,0) \ = \ \frac{\cosh\sigma(|x-y+1|-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} \ = \ \frac{\cosh\sigma(x-y+1-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma}$$

$$= \ \frac{\cosh\sigma(x-y+\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} \ = \ \frac{\cosh\sigma(y-x-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} \ = \ \frac{\cosh\sigma(|x-y|-\frac{1}{2})}{2\sigma\sinh\frac{1}{2}\sigma} \ = \ g(x,y)$$

set $c_j = g(x_j,0)h$, $j = 0 : N-1$, $0 \le x_j \le 1-h$

$$G_{jk} \ = \ g(x_j,x_k)h \ = \ \begin{cases} g(x_j-x_k,0)h & \text{if} \qquad 0 \le x_j - x_k \le 1-h \\ g(x_j-x_k+1,0)h & \text{if } \ -1+h \le x_j - x_k \le -h \end{cases}$$

$$= \begin{cases} c_{j-k} & \text{if } \ j-k = 0 : N-1 \\ c_{j-k+N} & \text{if } \ j-k = -N+1 : -1 \end{cases} \ = \ c_{(j-k)\mathrm{mod}N} \qquad \underline{\text{ok}}$$

$\Rightarrow G = F_N^* D F_N$, $D = \mathrm{diag}(\sqrt{N}\,\widehat{c}_n\,)$

$\Rightarrow u = Gf = F_N^* D F_N f \ : \ O(N\log N)$ ops

<u>particle systems</u>

example : charged particles in 3D

position : $x_j(t)$, $j = 1 : N$

charge : q_j , mass : m_j

configuration : $x(t) = (x_1(t), \ldots, x_N(t))^T$: molecule , beam , ...

Coulomb potential : $\phi(x) = \dfrac{1}{4\pi\epsilon_0|x|} \to \dfrac{1}{|x|}$

electric field : $E(x) = -\nabla\phi(x) = \dfrac{x}{|x|^3}$

dynamics : $m_i x_i'' = \displaystyle\sum_{\substack{j=1 \\ j\neq i}}^{N} q_i q_j \frac{x_i - x_j}{|x_i - x_j|^3}$, $i = 1 : N$

1. Direct summation requires $O(N^2)$ flops/timestep, but we will investigate faster methods.

2. These methods can also be applied to energy minimization.

$$V(x_1, \ldots, x_N) = \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{q_i q_j}{|x_i - x_j|} \ : \text{ electrostatic potential energy}$$

problem : find x^* such that $V(x^*) = \min\limits_x V(x)$

deterministic/Monte Carlo methods

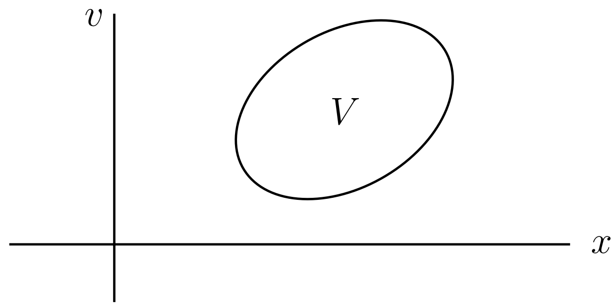
kinetic model

Consider a set of interacting particles that carry charge or mass.

$(x,v) \in \mathbb{R}^{2d}$, $d = 1,2,3$: phase space coordinates

$f(x,v,t)$: number density of particles in phase space

$N_V(t) = \int_V f(x,v,t)\,dx\,dv$: number of particles in volume V in phase space



In the absence of collisions and sources, particles can enter or leave the volume V only by crossing the boundary ∂V.

$U = (v,a)$: velocity of the phase fluid

v : velocity in x-direction

$a = a(x,v,t)$: acceleration = velocity in v-direction

$fU(x,v,t)$: particle flux in phase space

$$\frac{dN_V}{dt} = \frac{d}{dt}\int_V f(x,v,t)\,dx\,dv = \int_V f_t(x,v,t)\,dx\,dv = -\int_{\partial V} fU(x,v,t)\cdot dS$$
$$= -\int_V \nabla\cdot fU(x,v,t)\,dx\,dv$$

$\nabla = (\nabla_x, \nabla_v)$: gradient operator in phase space

$$\Rightarrow \int_V (f_t + \nabla\cdot fU)(x,v,t)\,dx\,dv = 0$$

$$\Rightarrow f_t + \nabla\cdot fU = 0 \;\Rightarrow\; f_t + \nabla_x\cdot(fv) + \nabla_v\cdot(fa) = 0$$

We consider conservative forces, i.e. $a = -\nabla\phi(x,t)$, hence $a = a(x,t)$.

$\Rightarrow f_t + v\cdot\nabla_x f + a\cdot\nabla_v f = 0$: Vlasov equation

Under these assumptions, the phase flow is <u>incompressible</u>.

pf : $\nabla \cdot U = (\nabla_x, \nabla_v) \cdot (v, a) = \nabla_x v + \nabla_v a = 0$ <u>ok</u>

<u>example</u> : electrons (one-species plasma)

q : charge , m : mass

$$f_t + v \cdot \nabla_x f + \frac{F}{m} \cdot \nabla_v f = 0$$

$F = q\, E(x,t)$: electrostatic force

$E(x,t) = -\nabla_x \phi(x,t)$: electric field , $\phi(x,t)$: electric potential

$-\nabla^2 \phi = \rho$: Poisson equation

$\rho = \rho(x,t) = q\, n(x,t) + \overline{\rho}$: charge density in physical space

$n(x,t) = \int_{\mathbb{R}^d} f(x,v,t)\, dv$: number density of electrons in physical space

$\overline{\rho}$: uniform background positive charge density (e.g. immobile ions)

<u>Vlasov-Poisson system in 1d</u> : $0 \le x \le 1$, PBC, $-\infty < v < \infty$

$$f_t + v f_x + \frac{F}{m} f_v = 0 \ , \ f(0,v,t) = f(1,v,t) \ , \ \lim_{v \to \pm\infty} f(x,v,t) = 0$$

$$F = q\, E(x,t) \ , \ E(x,t) = -\phi_x(x,t)$$

$$-\phi_{xx} = \rho \ , \ \phi(0,t) = \phi(1,t) \ , \ \phi_x(0,t) = \phi_x(1,t)$$

$$\rho = \rho(x,t) = q\, n(x,t) + \overline{\rho}$$

$$n(x,t) = \int_{-\infty}^{\infty} f(x,v,t)\, dv$$

<u>note</u>

$\int_0^1 \rho(x,t)\, dx = \int_0^1 -\phi_{xx}(x,t)\, dx = \phi_x(0,t) - \phi_x(1,t) = 0$: <u>charge neutrality</u>

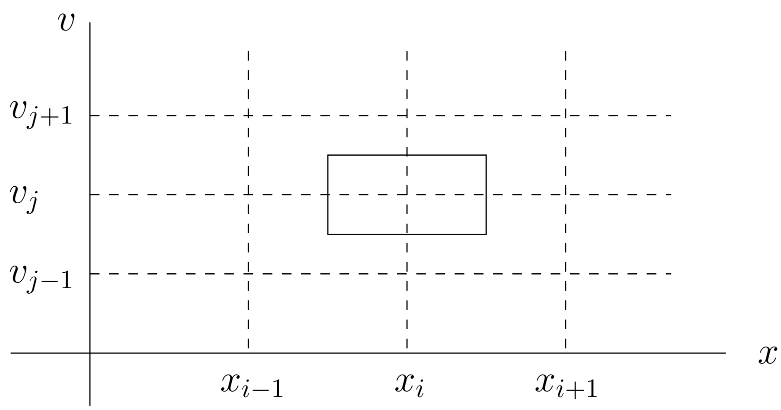
1. This condition is necessary and sufficient for existence of a solution $\phi(x,t)$; the background charge density $\overline{\rho}$ ensures it is satisfied.

2. If $\phi(x,t)$ is a solution, then so is $\phi(x,t) + c$ for any constant c, so the potential is not unique, but the field is unique.

numerical methods for Vlasov-Poisson in 1d

Vlasov-Poisson method 1 : finite-difference scheme

$x_i = i\Delta x$, $v_j = j\Delta v$: mesh in phase space , $t^n = n\Delta t$



$C_{ij} = \{(x,v) : x_{i-1/2} \le x < x_{i+1/2} , v_{j-1/2} \le v < v_{j+1/2}\}$: cell

$f_{ij}^n = f(x_i, v_j, t^n)$

$f_{ij}^n \,\Delta x\, \Delta v$ = number of particles in cell C_{ij} at time t^n

Lax-Friedrichs

$$f_t + v f_x + \frac{F}{m} f_v = 0$$

$$\frac{f_{ij}^{n+1} - \frac{1}{4}(f_{i+1,j}^n + f_{i-1,j}^n + f_{i,j+1}^n + f_{i,j-1}^n)}{\Delta t} + v_j D_0^x f_{ij}^n + \frac{F_i^n}{m} D_0^v f_{ij}^n = 0$$

$$D_0^x f_{ij}^n = \frac{f_{i+1,j}^n - f_{i-1,j}^n}{2\Delta x} \ , \ D_0^v f_{ij}^n = \frac{f_{i,j+1}^n - f_{i,j-1}^n}{2\Delta v}$$

$F_i^n = qE_i^n$, $E_i^n = -D_0^x \phi_i^n$

$-D_+^x D_-^x \phi_i^n = \rho_i^n$ + PBC : comment soon

$$\rho_i^n = q \sum_{j=-J}^{J} f_{ij}^n \,\Delta v + \overline{\rho}$$

1. CFL condition : $\Delta t \le \min\left\{\dfrac{\Delta x}{\max|v_j|} , \dfrac{\Delta v}{\max|F_i^n|/m}\right\}$

2. artificial diffusion/collisions

discrete Poisson equation in 1d with PBC

$$\frac{-\phi_{i+1}+2\phi_i-\phi_{i-1}}{\Delta x^2}=\rho_i \ , \ i=0:N-1 \ , \ \Delta x=1/N \ , \ \phi_{-1}=\phi_{N-1} \ , \ \phi_N=\phi_0$$

$$\frac{1}{\Delta x^2}\begin{pmatrix} 2 & -1 & \cdots & \cdots & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & \cdots & \cdots & -1 & 2 \end{pmatrix}\begin{pmatrix}\phi_0\\ \phi_1\\ \vdots \\ \phi_{N-2}\\ \phi_{N-1}\end{pmatrix}=\begin{pmatrix}\rho_0\\ \rho_1\\ \vdots \\ \rho_{N-2}\\ \rho_{N-1}\end{pmatrix}$$

1. adding all eqs $\Rightarrow \sum_{i=0}^{N-1}\rho_i=0$: discrete charge neutrality

2. if $\{\phi_i\}_{i=0}^{N-1}$ is a solution, then so is $\{\phi_i+c\}_{i=0}^{N-1}$ for any constant c

This is analogous to the continuous case.

method 1a : spectral

$A\phi=\rho$, $A=F_N^*DF_N$, $D=\mathrm{diag}(\lambda_0,\ldots,\lambda_{N-1})$

e-values : $\lambda_n=\dfrac{4\sin^2(\pi n/N)}{\Delta x^2}$, $n=0:N-1$

e-vectors : $q_n=F_N^*e_n=\dfrac{1}{\sqrt{N}}(1,\omega^{-n},\omega^{-2n},\ldots,\omega^{-(N-1)n})^T$, $\omega=e^{-2\pi i/N}$

note : $\lambda_0=0 \Rightarrow A$ is not invertible , $\mathrm{null}(A)=\mathrm{span}(q_0)$, $q_0=\dfrac{1}{\sqrt{N}}(1,\ldots,1)^T$

then $A\phi=\rho$ has a solution $\Leftrightarrow \rho$ is orthogonal to $\mathrm{null}(A^*)$

$\Leftrightarrow \langle\rho,q_0\rangle=\dfrac{1}{\sqrt{N}}\sum_{i=0}^{N-1}\rho_i=0$: discrete charge neutrality

Moreover, if ϕ is a solution, then so is $\phi+cq_0$ for any constant c.

claim: Let $\phi=F_N^*D^{-1}F_N\rho$, where $D^{-1}=\mathrm{diag}(0,\lambda_1^{-1},\ldots,\lambda_{N-1}^{-1})$ and ρ satisfies discrete charge neutrality, Then $A\phi=\rho$.

pf :
$$\begin{aligned} A\phi &= F_N^*DF_NF_N^*D^{-1}F_N\rho = F_N^*\,\mathrm{diag}(0,1,\ldots,1)F_N\rho \\ &= F_N^*\,\mathrm{diag}(1,1,\ldots,1)F_N\rho = \rho \end{aligned}$$

$(F_N\rho)_0=\langle F_N\rho,e_0\rangle=\langle\rho,F_N^*e_0\rangle=\langle\rho,q_0\rangle=0$ ok

note : $O(N\log N)$ flops

<u>method 1b</u> : elimination

set $\phi_0 = 0$, write down eqs for $i = 1 : N-1$, then eq for $i = 0$

$$\begin{aligned}
&2\phi_1 - \phi_2 &&= \rho_1 \Delta x^2 \\
&-\phi_1 + 2\phi_2 - \phi_3 &&= \rho_2 \Delta x^2 \\
&\qquad -\phi_2 + 2\phi_3 - \phi_4 &&= \rho_3 \Delta x^2 \\
& &&\vdots \\
&\qquad\qquad -\phi_{N-3} + 2\phi_{N-2} - \phi_{N-1} &&= \rho_{N-2} \Delta x^2 \\
&\qquad\qquad\qquad -\phi_{N-2} + 2\phi_{N-1} &&= \rho_{N-1} \Delta x^2 \\
&-\phi_1 \qquad\qquad\qquad\qquad - \phi_{N-1} &&= \rho_N \Delta x^2 \ , \ \text{set } \rho_N = \rho_0
\end{aligned}$$

multiply 1st eq by 1, 2nd eq by 2, ..., Nth eq by N, then add

$$\Rightarrow -N\phi_1 = \sum_{i=1}^{N} i\rho_i \Delta x^2$$

check : for $i = 2 : N-1$, coeff of ϕ_i is $-(i-1) + 2i - (i+1) = 0$

solve for ϕ_1, then ϕ_2, then ϕ_3, ..., then ϕ_{N-1}

to show Nth eq is satisfied : add all eqs, ok by discrete charge neutrality

note : $O(N)$ flops

<u>Vlasov-Poisson method 2</u> : particle-in-cell (PIC)

idea : convect particles in phase space, solve Poisson equation on a mesh

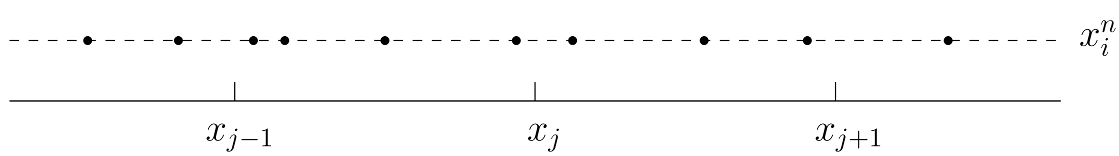
particles : $x_i(t)$, $v_i(t)$, $i = 1 : N_p$, charge q , mass $m = 1$

Newton's equation : $x_i' = v_i$, $v_i' = F(x_i)$

leap-frog method : $\dfrac{x_i^{n+1} - x_i^n}{\Delta t} = v_i^{n+1/2}$, $\dfrac{v_i^{n+1/2} - v_i^{n-1/2}}{\Delta t} = F_i^n$

$t^n = n\Delta t$, $t^{n+1/2} = (n + \frac{1}{2})\Delta t$

mesh : $x_j = j\Delta x$, $\Delta x = 1/N_m$, $j = 0 : N_m$



$-D_+^x D_-^x \phi_j^n = \rho_j^n$ + PBC , $E_j^n = -D_0^x \phi_j^n$, $F_j^n = qE_j^n$

<u>one time step</u>

input : x_i^n , $v_i^{n-1/2}$ $\to$ output : x_i^{n+1} , $v_i^{n+1/2}$, $i = 1 : N_p$

1. <u>assign charge</u> from particles to mesh : $x_i^n \to \rho_j^n$
2. solve Poisson equation for potential on mesh : $\rho_j^n \to \phi_j^n$
3. compute forces on mesh : $\phi_j^n \to F_j^n$
4. <u>interpolate forces</u> from mesh to particles : $F_j^n \to F_i^n$
5. convect particles in phase space : $F_i^n \to x_i^{n+1}, v_i^{n+1/2}$

<u>nearest mesh point scheme</u> : NMP

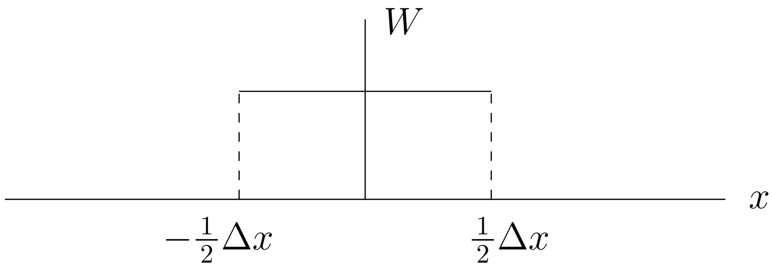
cell j : $x_{j-1/2} \le x < x_{j+1/2}$

charge assignment : $\rho_j^n = \dfrac{q\, n_j^n}{\Delta x} + \overline{\rho}$, n_j^n : number of particles in cell j at time t^n

force interpolation : if particle x_i^n is in cell j , set $F_i^n = F_j^n$

NMP has low accuracy, but there is an alternative viewpoint that can be used to derive more accurate schemes.

define : $W(x) = \begin{cases} 1 \text{ if } -\frac{1}{2}\Delta x \le x < \frac{1}{2}\Delta x \\ 0 \text{ otherwise} \end{cases}$: weight function



$$\rho_j^n = \frac{q\, n_j^n}{\Delta x} + \overline{\rho} \ , \ n_j^n = \sum_{i=1}^{N_p} W(x_i^n - x_j) \ , \ F_i^n = \sum_{j=0}^{N_m-1} W(x_i^n - x_j) F_j^n$$

note : assume $-\frac{1}{2}\Delta x \le x_i^n < 1 - \frac{1}{2}\Delta x$ by PBC

<u>code 1</u> : $O(N_m N_p)$ flops

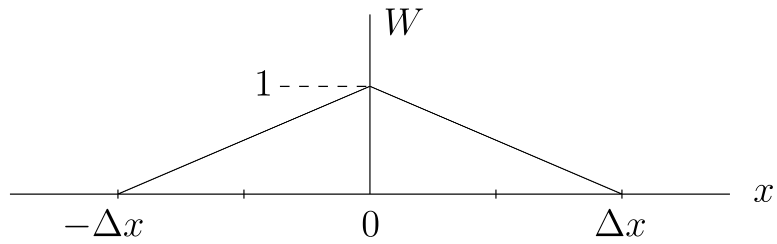
```
for j = 0 : N_m - 1
   n_j^n = 0
   for i = 1 : N_p
      n_j^n = n_j^n + W(x_i^n - x_j)
   end
end
```

<u>code 2</u> : $O(N_m + N_p)$ flops

```
for j = 0 : N_m - 1
   n_j^n = 0
end
for i = 1 : N_p
   j = integer_part((x_i^n + 1/2 Δx)/Δx)
   n_j^n = n_j^n + 1
end
```

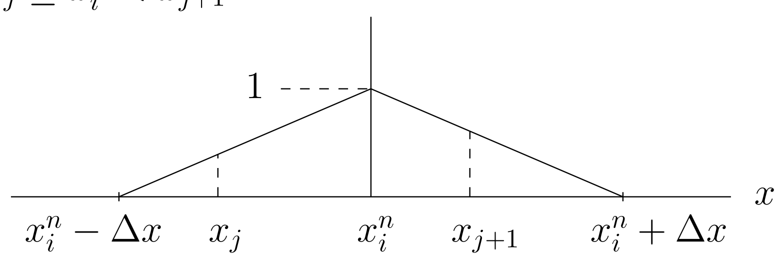
cloud-in-cell scheme : CIC

$$W(x) = \begin{cases} 1 - |x|/\Delta x & \text{if } -\Delta x \le x < \Delta x \\ 0 & \text{otherwise} \end{cases}$$



force interpolation : $F_i^n = \sum_{j=0}^{N_m-1} W(x_j - x_i^n) F_j^n$

assume $x_j \le x_i^n < x_{j+1}$



$\Rightarrow\ F_i^n = W(x_j - x_i^n)F_j^n + W(x_{j+1} - x_i^n)F_{j+1}^n = c_1 F_j^n + c_2 F_{j+1}^n$

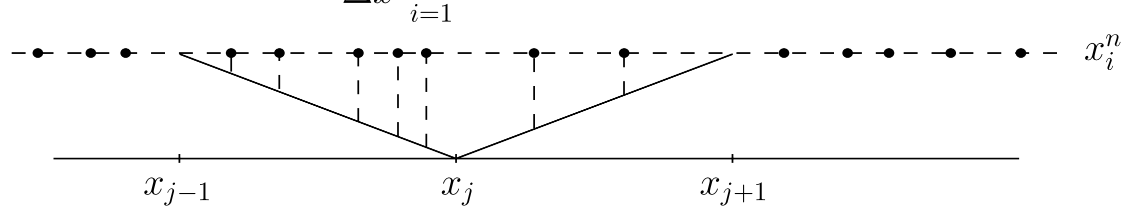
$$c_1 = W(x_j - x_i^n) = 1 - \frac{|x_j - x_i^n|}{\Delta x} = \frac{\Delta x - (x_i^n - x_j)}{\Delta x} = \frac{x_{j+1} - x_i^n}{\Delta x}$$

$$c_2 = W(x_{j+1} - x_i^n) = 1 - \frac{|x_{j+1} - x_i^n|}{\Delta x} = \frac{\Delta x - (x_{j+1} - x_i^n)}{\Delta x} = \frac{x_i^n - x_j}{\Delta x}$$

$0 \le c_1\,,\ c_2 \le 1\ ,\ c_1 + c_2 = 1$

$\Rightarrow F_i^n$ is a distance-weighted average of the force at the 2 nearest mesh points

charge assignment : $\rho_j^n = \frac{q}{\Delta x} \sum_{i=1}^{N_p} W(x_i^n - x_j) + \overline{\rho}$



$\Rightarrow \rho_j^n$ is a distance-weighted average of the particle charge in the 2 nearest cells

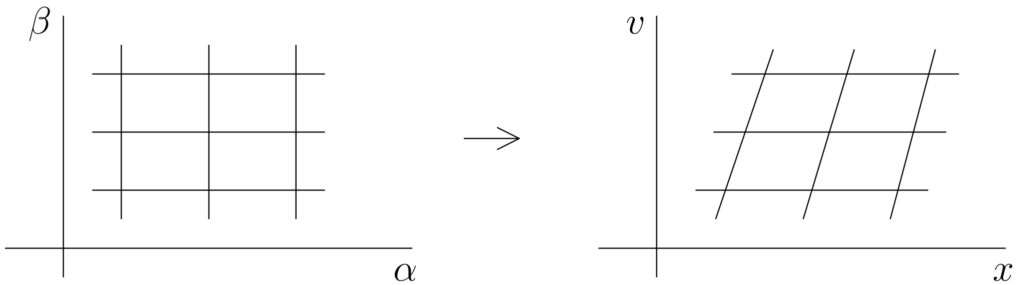
The CIC weight function is continuous and this leads to higher order accuracy.

<u>Vlasov-Poisson method 3</u> : integral based particle method

recall : $f_t + vf_x + Ff_v = 0$, $F = qE$, $E = -\phi_x$, $-\phi_{xx} = \rho$, PBC

$$\rho = \rho(x,t) = q\int_{-\infty}^{\infty} f(x,v,t)\,dv + \overline{\rho} \text{ , charge neutrality}$$

define : $\begin{pmatrix}\alpha\\ \beta\end{pmatrix} \to \begin{pmatrix}x(\alpha,\beta,t)\\ v(\alpha,\beta,t)\end{pmatrix}$: <u>flow map</u> of particle distribution



(α,β) : <u>Lagrangian coordinates</u> , particle labels

Newton's equation : $x_t(\alpha,\beta,t) = v(\alpha,\beta,t)$, $v_t(\alpha,\beta,t) = F(x(\alpha,\beta,t))$

initial conditions : $x(\alpha,\beta,0) = \alpha$, $v(\alpha,\beta,0) = \beta$

PBC : $x(\alpha+1,\beta,t) = x(\alpha,\beta,t) + 1$, $v(\alpha+1,\beta,t) = v(\alpha,\beta,t)$

<u>claim</u>

1. $f(x(\alpha,\beta,t), v(\alpha,\beta,t), t) = f(\alpha,\beta,0)$

2. $J(\alpha,\beta,t) = \det\begin{pmatrix}x_\alpha(\alpha,\beta,t) & x_\beta(\alpha,\beta,t)\\ y_\alpha(\alpha,\beta,t) & y_\beta(\alpha,\beta,t)\end{pmatrix} \Rightarrow J(\alpha,\beta,t) = J(\alpha,\beta,0) = 1$

<u>pf</u>

1. $\dfrac{d}{dt}f(x(\alpha,\beta,t), v(\alpha,\beta,t), t) = f_x x_t + f_v v_t + f_t = f_x v + f_v F + f_t = 0$ <u>ok</u>

Hence $f(x,v,t)$ is constant on the <u>characteristics</u> of the Vlasov equation.

2. $J(t+h) = \det\begin{pmatrix}x_\alpha(t+h) & x_\beta(t+h)\\ v_\alpha(t+h) & v_\beta(t+h)\end{pmatrix}$

$$= \det\begin{pmatrix}x_\alpha + hx_{\alpha t} + O(h^2) & x_\beta + hx_{\beta t} + O(h^2)\\ v_\alpha + hv_{\alpha t} + O(h^2) & v_\beta + hv_{\beta t} + O(h^2)\end{pmatrix}$$

$$= (x_\alpha v_\beta - v_\alpha x_\beta) + h(x_\alpha v_{\beta t} + x_{\alpha t} v_\beta - (v_\alpha x_{\beta t} + v_{\alpha t} x_\beta)) + O(h^2)$$

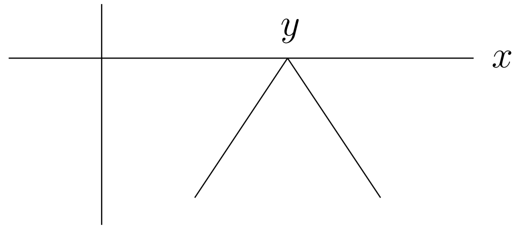
$$= J(t) + h(x_\alpha F_x x_\beta + v_\alpha v_\beta - (v_\alpha v_\beta + F_x x_\alpha x_\beta)) + O(h^2) = J(t) + O(h^2)$$

$\Rightarrow J'(t) = \lim\limits_{h\to 0}\dfrac{J(t+h) - J(t)}{h} = 0$ <u>ok</u>

integral expression for $\phi(x,t)$

$g(x,y) \;=\; -\frac{1}{2}|x-y|$: free-space Green's function in 1d

$$= \begin{cases} -\frac{1}{2}(x-y) \text{ if } x > y \\ \ \frac{1}{2}(x-y) \text{ if } x < y \end{cases}$$



1. $-g_{xx}(x,y) = 0$ for $x \neq y$, $g(x,x^-) = g(x,x^+)$, $g_x(x,x^-) - g_x(x,x^+) = -1$

This is equivalent to saying $-g_{xx}(x,y) = \delta(x-y)$, i.e. $g(x,y)$ is the potential of a point charge at $x = y$.

2. $\phi = \phi_p + \phi_h$, $\phi_p(x,t) = \displaystyle\int_0^1 g(x,y)\rho(y,t)dy$, $\phi_h(x,t) = ax + b$

3. PBC

Since $\phi(x,t)$ is determined up to an additive constant, we choose $b = 0$.

$$\phi_x(1,t) - \phi_x(0,t) = \int_0^1 \phi_{xx}(x,t)dx = \int_0^1 -\rho(x,t)dx = 0 \text{ by charge neutrality}$$

$$\phi(0,t) = \phi(1,t) \Rightarrow \phi_p(0,t) + \phi_h(0,t) = \phi_p(1,t) + \phi_h(1,t) \Rightarrow \phi_p(0,t) = \phi_p(1,t) + a$$

$$a = \phi_p(0,t) - \phi_p(1,t) = \int_0^1 \underbrace{\big(g(0,y) - g(1,y)\big)}_{-\frac{1}{2}y - (-\frac{1}{2}(1-y)) = \frac{1}{2} - y}\rho(y,t)dy = \int_0^1 \big(\tfrac{1}{2} - y\big)\rho(y,t)dy$$

$$\Rightarrow a = -\int_0^1 y\rho(y,t)dt \text{ by charge neutrality}$$

$$\Rightarrow \phi(x,t) = \int_0^1 \big(g(x,y) - xy\big)\rho(y,t)dy \ , \text{ check : hw3}$$

This generalizes to 2d and 3d using the free-space Green's function for ϕ_p, and a boundary integral representation for ϕ_h.

force evaluation : $F(x(\alpha,\beta,t))$

$$E(x,t) = -\phi_x(x,t) = \int_0^1 (-g_x(x,y) + y)\rho(y,t)dy \ , \ g_x(x,y) = -\tfrac{1}{2}\text{sign}(x-y)$$

$$= \int_0^1 (-g_x(x,y) + y)\left(q\int_{-\infty}^{\infty} f(y,v,t)dv + \overline{\rho}\right)dy$$

x : hw3

$$= \int_0^1\int_{-\infty}^{\infty} q(-g_x(x,y) + y)f(y,v,t)dvdy \ + \ \cancel{\overline{\rho}\int_0^1 (-g_x(x,y) + y)dy}$$

$$E(x,t) = \int_{-\infty}^{\infty}\int_0^1 q(-g_x(x,y)+y)f(y,v,t)dydv + \overline{\rho}\,x\int_{-\infty}^{\infty}\int_0^1 f(y,v,t)dydv$$

$$= \int_{-\infty}^{\infty}\int_0^1 \big(q(-g_x(x,y)+y)+\overline{\rho}x\big)f(y,v,t)dvdy$$

$$= \int_{-\infty}^{\infty}\int_0^1 k(x,y)f(y,v,t)dvdy\ ,\ \ k(x,y) = q(-g_x(x,y)+y)+\overline{\rho}x$$

change variables by flow map : $(y,v) \to (x(\alpha,\beta,t), v(\alpha,\beta,t))$

$$E(x,t) = \int_{-\infty}^{\infty}\int_0^1 k(x,x(\alpha,\beta,t))f(x(\alpha,\beta,t),v(\alpha,\beta,t),t)J(\alpha,\beta,t)d\alpha d\beta$$

$$= \int_{-\infty}^{\infty}\int_0^1 k(x,x(\alpha,\beta,t))f_0(\alpha,\beta)d\alpha d\beta$$

<u>summary</u> : integro-differential equation for the flow map

$x_t(\alpha,\beta,t) = v(\alpha,\beta,t)$

$v_t(\alpha,\beta,t) = F(x(\alpha,\beta,t)) = q\int_{-\infty}^{\infty}\int_0^1 k(x(\alpha,\beta,t),x(\tilde\alpha,\tilde\beta,t))f_0(\tilde\alpha,\tilde\beta)d\tilde\alpha d\tilde\beta$

<u>discretization</u> : $(\alpha,\beta)\ \to\ (\alpha_i,\beta_i)\ ,\ i = 1:N$

$x(\alpha_i,\beta_i,t)\,,\,v(\alpha_i,\beta_i,t)\ \to\ x_i(t)\,,\,v_i(t)$: particles in phase space

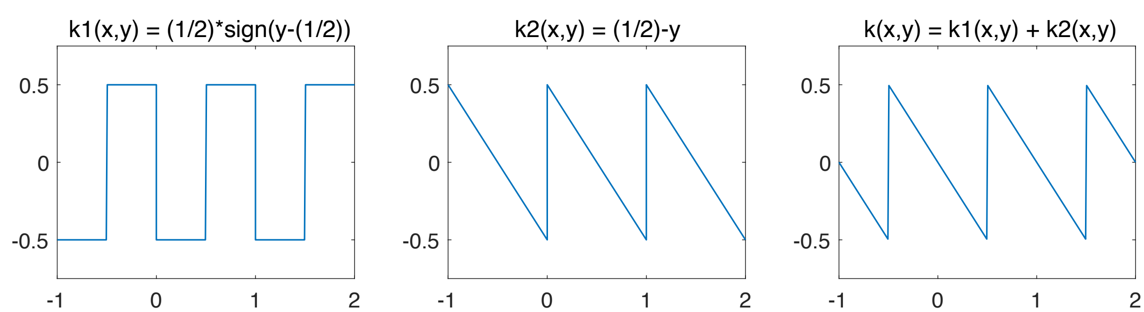
$$x_i' = v_i\ ,\ \ v_i' = F(x_i) = q\sum_{j=1}^{N} k(x_i,x_j)f_0(\alpha_j,\beta_j)\Delta\alpha\,\Delta\beta$$

This is a finite-dimensional system of ODEs, but there are 3 issues.

1. The particle distribution becomes disordered.
2. Evaluating the RHS by direct summation requires $O(N^2)$ flops/timestep.
3. The electric field kernel $k(x,y)$ is singular for $x = y$.

example : $q = -1\,,\ \overline{\rho} = 1\,,\ x = \frac{1}{2}$

$k(x,y) = q(-g_x(x,y)+y)+\overline{\rho}x = \frac{1}{2}\mathrm{sign}(y-\frac{1}{2}) + (\frac{1}{2}-y)$



fluid dynamics in 2d

$\vec{u} = (u, v)$: velocity field , $u = u(x, y, t)$, $v = v(x, y, t)$

We consider incompressible flow, i.e. $u_x + v_y = 0$.

1. An incompressible flow is area-preserving.

2. If (u, v) is incompressible, then there exists a stream function, $\psi(x, y)$, such that $u = \psi_y$, $v = -\psi_x$.

note : If ψ exists, then $u_x + v_y = (\psi_y)_x + (-\psi_x)_y = 0$.

def : A streamline is a level curve of the stream function, i.e. $\psi(x, y) = c$.

claim : The velocity field is parallel to the streamlines.

pf

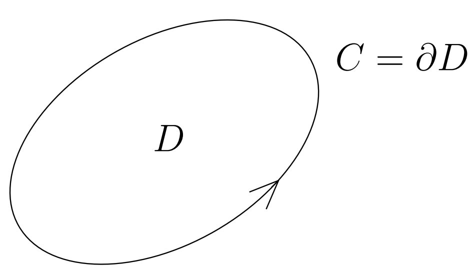
$(x(s), y(s))$: streamline $\Rightarrow \psi(x(s), y(s)) = c \Rightarrow \psi_x \cdot x' + \psi_y \cdot y' = 0$

$\Rightarrow -v \cdot x' + u \cdot y' = 0 \Rightarrow (u, v) \cdot (y', -x') = 0 \Rightarrow (u, v) \cdot (x', y')^\perp = 0$ ok

def : $\omega = v_x - u_y$: vorticity , units $= T^{-1}$

interpretation

Consider the line integral of the velocity around a closed curve C bounding a domain D.



$$\int_C \vec{u} \cdot ds \ : \ \text{circulation}$$

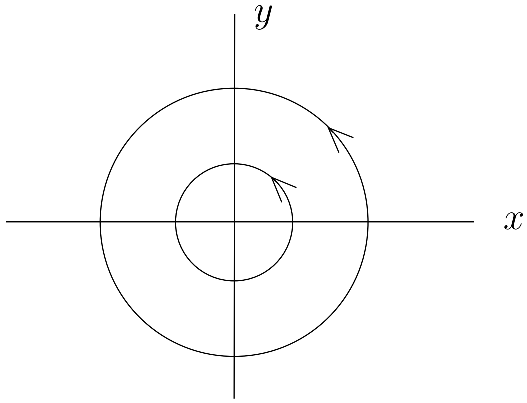
$$\int_C \vec{u} \cdot ds = \int_{\partial D} u\,dx + v\,dy = \int_D (v_x - u_y)\,dx\,dy = \int_D \omega\,dx\,dy$$

$\Rightarrow$ vorticity = circulation density = local rotation rate

note : $\omega = v_x - u_y = (-\psi_x)_x - (\psi_y)_y \Rightarrow -\nabla^2\psi = \omega$: Poisson equation

<u>example</u> : point vortex

$\psi(x,y) = -\frac{1}{2\pi}\ln r$, $r = \sqrt{x^2+y^2}$ $\Rightarrow$ streamlines are circles



$$u(x,y) = \frac{-y}{2\pi(x^2+y^2)} \ , \ v(x,y) = \frac{x}{2\pi(x^2+y^2)} \Rightarrow \sqrt{u^2+v^2} = \frac{1}{2\pi r}$$

$$\omega = -\nabla^2\psi = -\left(\psi_{rr} + \frac{1}{r}\psi_r + \frac{1}{r^2}\psi_{\theta\theta}\right) = \frac{1}{2\pi}\left(-\frac{1}{r^2} + \frac{1}{r}\cdot\frac{1}{r}\right) = 0 \ , \ \text{if } r \neq 0$$

However, consider the circulation around a circle of radius R.

C : $x = R\cos\theta$, $y = R\sin\theta$, $0 \le \theta \le 2\pi$

$$\int_C \vec{u}\cdot ds = \int_C u\,dx + v\,dy = \int_0^{2\pi}\left(\frac{-R\sin\theta}{2\pi R^2}\cdot -R\sin\theta + \frac{R\cos\theta}{2\pi R^2}\cdot R\cos\theta\right)d\theta$$

$$= \frac{1}{2\pi}\int_0^{2\pi} d\theta = 1 \ : \ \text{independent of } R \ , \ \text{but recall : } \int_C \vec{u}\cdot ds = \int_D \omega dxdxy$$

<u>claim</u> : The vorticity associated with a point vortex is a delta function, i.e. if $\psi = -\frac{1}{2\pi}\ln r$, then $\omega = -\nabla^2\psi = \delta$ in the <u>sense of distributions</u>.

notation : $<f,g> = \int_{\mathbb{R}^2} f(x,y)\,g(x,y)\,dx\,dy$

<u>def</u> : The delta function $\delta(x,y)$ is the distribution satisfying

$$<\delta,f> = \int_{\mathbb{R}^2}\delta(x,y)\,f(x,y)\,dx\,dy = f(0,0) \text{ for all } \underline{\text{test functions}}\ f \in C_0^\infty(\mathbb{R}^2).$$

The <u>weak form</u> of the equation $-\nabla^2\psi = \delta$ says that $<-\nabla^2\psi, f> = <\delta, f>$ for all test functions f, where $<-\nabla^2\psi, f> = <\psi, -\nabla^2 f>$ by definition, hence we must show that $<\psi, -\nabla^2 f> = f(0,0)$.

$$\underline{\text{pf}} : <-\nabla^2\psi, f> = <\psi, -\nabla^2 f> = \int_0^{2\pi}\int_0^{\infty} \psi(r) \cdot -\left(\frac{1}{r}\big(rf_r\big)_r + \frac{1}{r^2} f_{\theta\theta}\right) r\,dr\,d\theta$$

$$= \frac{1}{2\pi}\int_0^{2\pi}\int_0^{\infty} \ln r \cdot \big(rf_r\big)_r \,dr\,d\theta + \frac{1}{2\pi}\int_0^{2\pi}\int_0^{\infty} \ln r \cdot \frac{1}{r} f_{\theta\theta}\,dr\,d\theta$$

$$= \frac{1}{2\pi}\int_0^{2\pi}\left(\cancel{\ln r \cdot r f_r \Big|_{r=0}^{r=\infty}} - \int_0^{\infty} \frac{1}{r} \cdot r f_r\,dr\right) d\theta + \frac{1}{2\pi}\int_0^{\infty}\left(\ln r \cdot \frac{1}{r}\int_0^{2\pi} f_{\theta\theta}\,d\theta\right) dr$$

$$= -\frac{1}{2\pi}\int_0^{2\pi}\int_0^{\infty} f_r\,dr\,d\theta + \frac{1}{2\pi}\int_0^{\infty} \ln r \cdot \frac{1}{r} \cdot \cancel{f_\theta \Big|_{\theta=0}^{\theta=2\pi}}\,dr$$

$$= -\frac{1}{2\pi}\int_0^{2\pi} f \Big|_{r=0}^{r=\infty} d\theta = -\frac{1}{2\pi}\int_0^{2\pi} -f(0,0)\,d\theta = f(0,0) = <\delta, f> \quad \underline{\text{ok}}$$

---

1. A function satisfying $-\nabla^2 g = \delta$ is called a Green's function for the Laplace operator; the RHS represents a point vortex/charge/mass and g is the corresponding stream function/potential.

2. We've shown that $g(x,y) = -\frac{1}{2\pi}\ln(x^2+y^2)^{1/2}$ is a Green's function for the Laplace operator in 2d; in 3d a Green's function is $g(x,y,z) = \frac{1}{4\pi}(x^2+y^2+z^2)^{-1/2}$. (hw3)

3. If g is a Green's function and h is harmonic, i.e. $\nabla^2 h = 0$, then $g+h$ is also a Green's function. In any given BVP, the BC specify the Green's function.

4. For a general incompressible velocity field, the Poisson equation for the stream function, $-\nabla^2\psi = \omega$, can be solved by convolution.

$$\psi(x,y) = (g*\omega)(x,y) = \int_{\mathbb{R}^2} g(x-\widetilde{x}, y-\widetilde{y})\,\omega(\widetilde{x},\widetilde{y})\,d\widetilde{x}\,d\widetilde{y}$$

check : $-\nabla^2\psi = -\nabla^2(g*\omega) = (-\nabla^2 g)*\omega = \delta*\omega = \omega$ <u>ok</u>

5. This yields an integral expression for the velocity.

$\psi = g*\omega \;\Rightarrow\; (u,v) = (\psi_y, -\psi_x) = (g_y*\omega, -g_x*\omega)$

$$u(x,y) = \frac{1}{2\pi}\int_{\mathbb{R}^2} \frac{-(y-\widetilde{y})}{(x-\widetilde{x})^2+(y-\widetilde{y})^2}\omega(\widetilde{x},\widetilde{y})\,d\widetilde{x}\,d\widetilde{y}$$

$$v(x,y) = \frac{1}{2\pi}\int_{\mathbb{R}^2} \frac{(x-\widetilde{x})}{(x-\widetilde{x})^2+(y-\widetilde{y})^2}\omega(\widetilde{x},\widetilde{y})\,d\widetilde{x}\,d\widetilde{y}$$

In electromagnetic theory this is called the <u>Biot-Savart law</u>, where ω is a current density and (u,v) is the induced magnetic field.

question : In general $\omega = \omega(x,y,t)$; how does it evolve?

<u>2d incompressible Euler equations</u>

$\vec{u}_t + (\vec{u}\cdot\nabla)\vec{u} = -\nabla p$, $\nabla\cdot\vec{u} = 0$: velocity/pressure

$u_t + uu_x + vu_y = -p_x \Rightarrow u_{yt} + uu_{xy} + u_y u_x + vu_{yy} + v_y u_y = -p_{xy}$

$v_t + uv_x + vv_y = -p_y \Rightarrow v_{xt} + uv_{xx} + u_x v_x + vv_{xy} + v_x v_y = -p_{xy}$

$(u_y - v_x)_t + u(u_y - v_x)_x + v(u_y - v_x) + u_y(\cancel{u_x + v_y}) - v_x(\cancel{u_x + v_y}) = 0$

$\omega_t + u\omega_x + v\omega_y = 0$, $-\nabla^2\psi = \omega$, $u = \psi_y$, $v = -\psi_x$: vorticity/stream function

recall 1d Vlasov-Poisson

$f_t + vf_x + Ff_v = 0$, $-\phi_{xx} = \rho = q\displaystyle\int_{-\infty}^{\infty} f(x,v,t)\,dv + \overline{\rho}$, $F = -q\phi_x$

Similar considerations hold for these two systems, e.g. flow map, conservation, numerical methods (the analog of PIC is VIC = vortex-in-cell).

<u>integral based particle method</u>

$(x_i(t), y_i(t))$, $i = 1 : N$

discretize the Biot-Savart law , $\omega(x,y,t)dxdy \approx \omega(x_i,y_i,t)\Delta x\Delta y = \Gamma_i$

$$\frac{dx_i}{dt} = \frac{1}{2\pi}\sum_{j=1}^{N} \frac{-(y_i - y_j)}{(x_i - x_j)^2 + (y_i - y_j)^2 + \delta^2}\,\Gamma_j \quad , \quad \delta \ : \ \text{smoothing parameter}$$

$$\frac{dy_i}{dt} = \frac{1}{2\pi}\sum_{j=1}^{N} \frac{(x_i - x_j)}{(x_i - x_j)^2 + (y_i - y_j)^2 + \delta^2}\,\Gamma_j$$

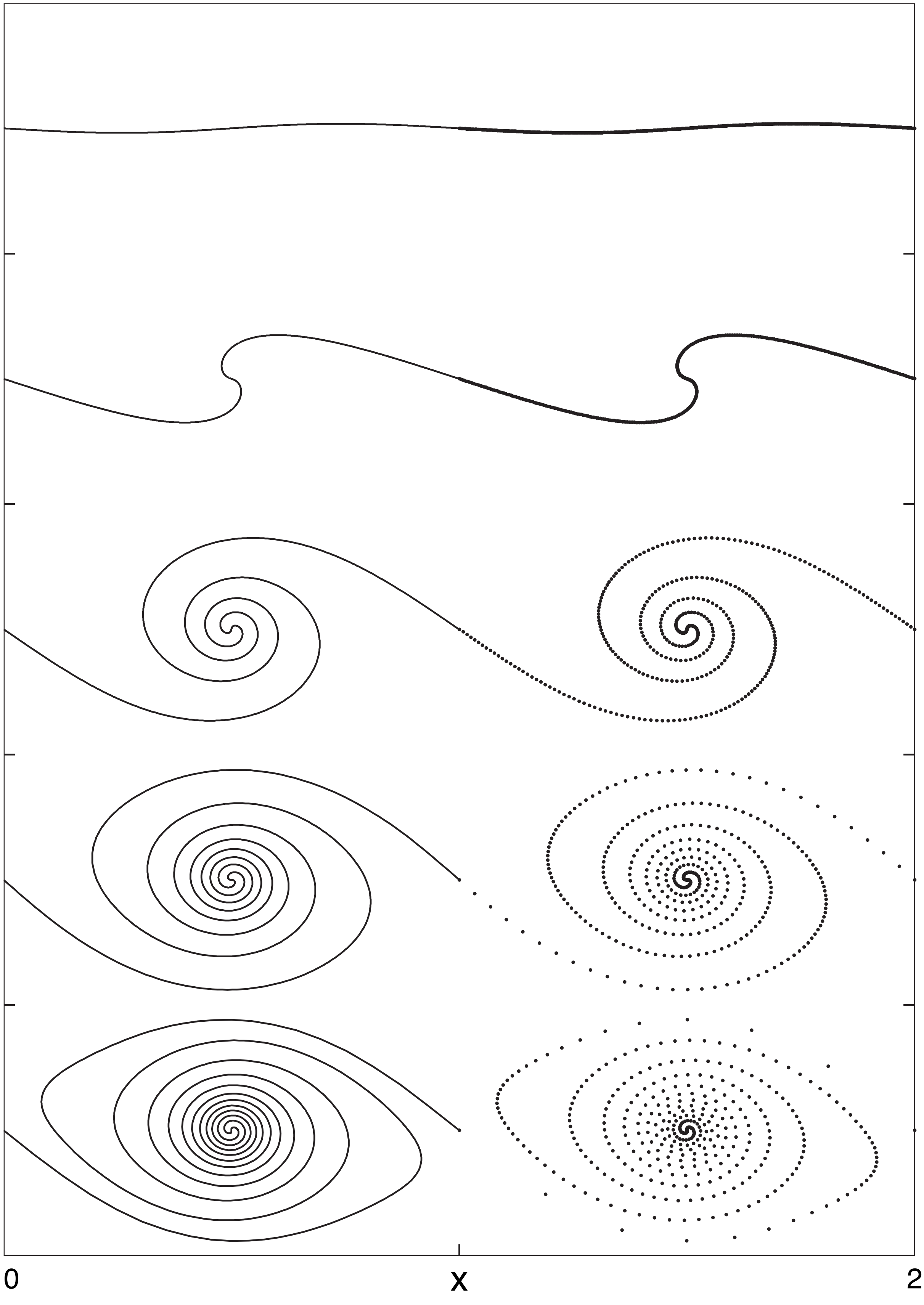
1. If $\delta = 0$ and we take $j \neq i$, then these are the <u>point vortex equations</u>.

2. We can think of the case $\delta > 0$ as arising from a regularized Green's function, $g_\delta(x,y) = -\frac{1}{2\pi}\ln(x^2 + y^2 + \delta^2)^{1/2}$; then each particle carries a smooth vorticity distribution called a <u>vortex-blob</u>.

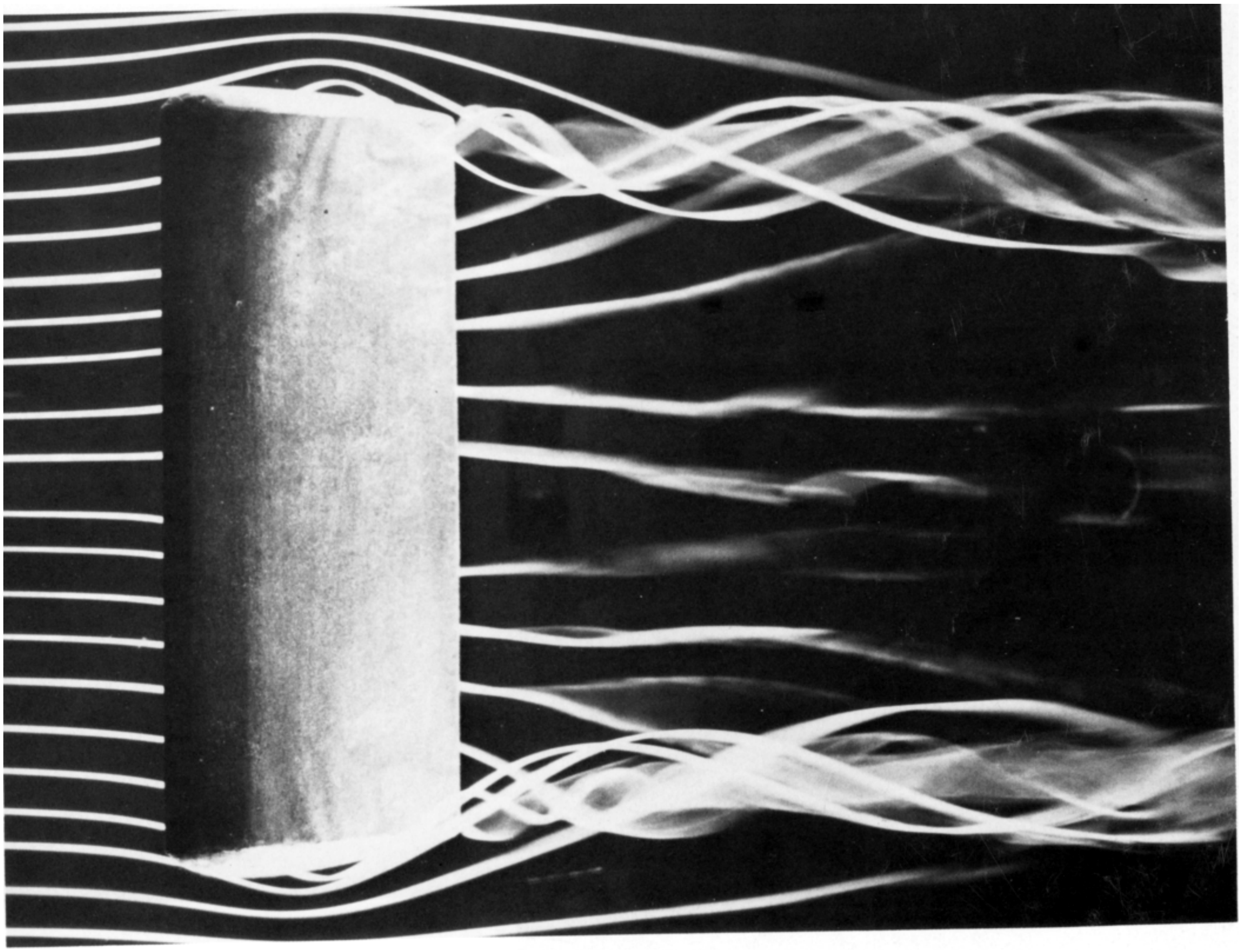
3. The vortex-blob method has no mesh-related artifacts such as artificial diffusion, but it does have artificial smoothing.

4. The vortex-blob method requires $O(N^2)$ flops/timestep if direct summation is used, but the cost can be reduced to $O(N\log N)$ using a treecode.

periodic vortex sheet roll-up/Kelvin-Helmholtz instability ($N = 400\,,\delta = 0.25$)



tip vortices/airfoil wake



vortex sheet model of an airplane wake (Prandtl)

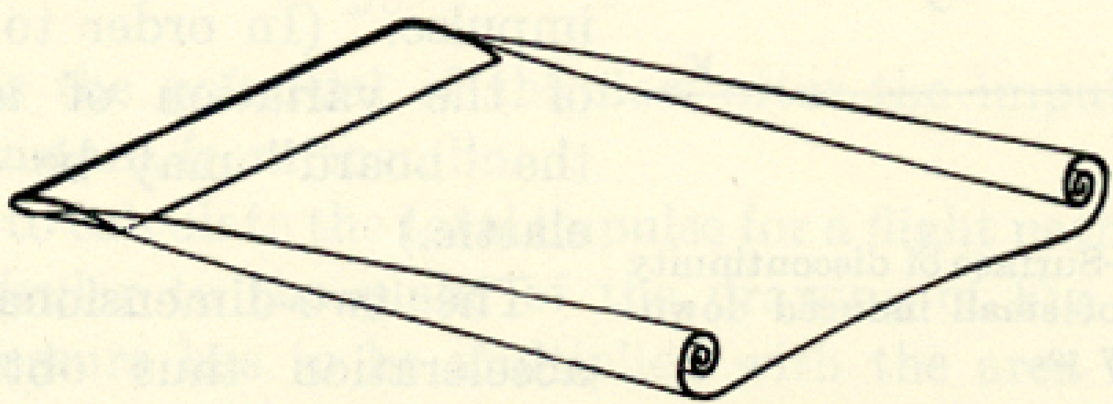
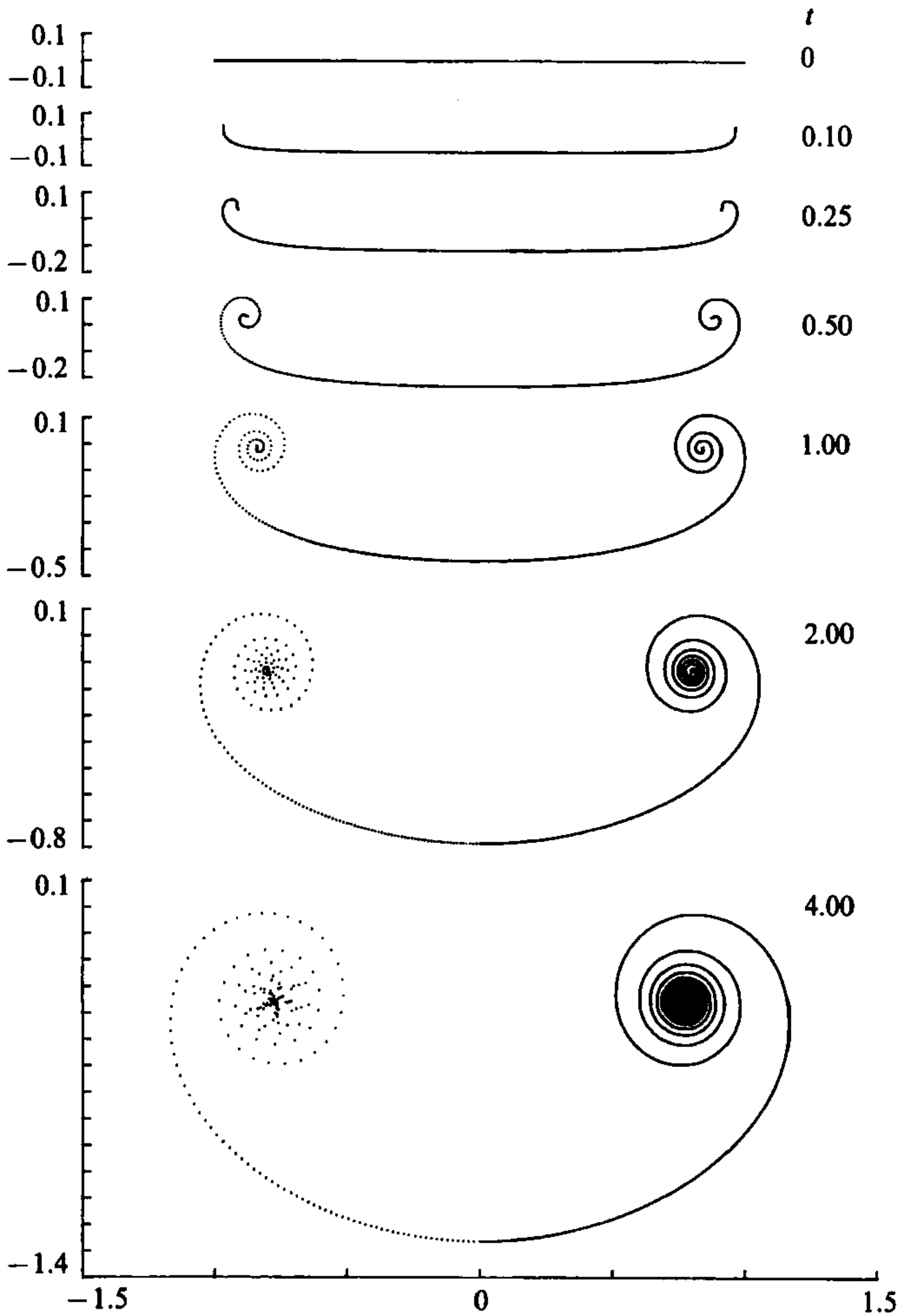
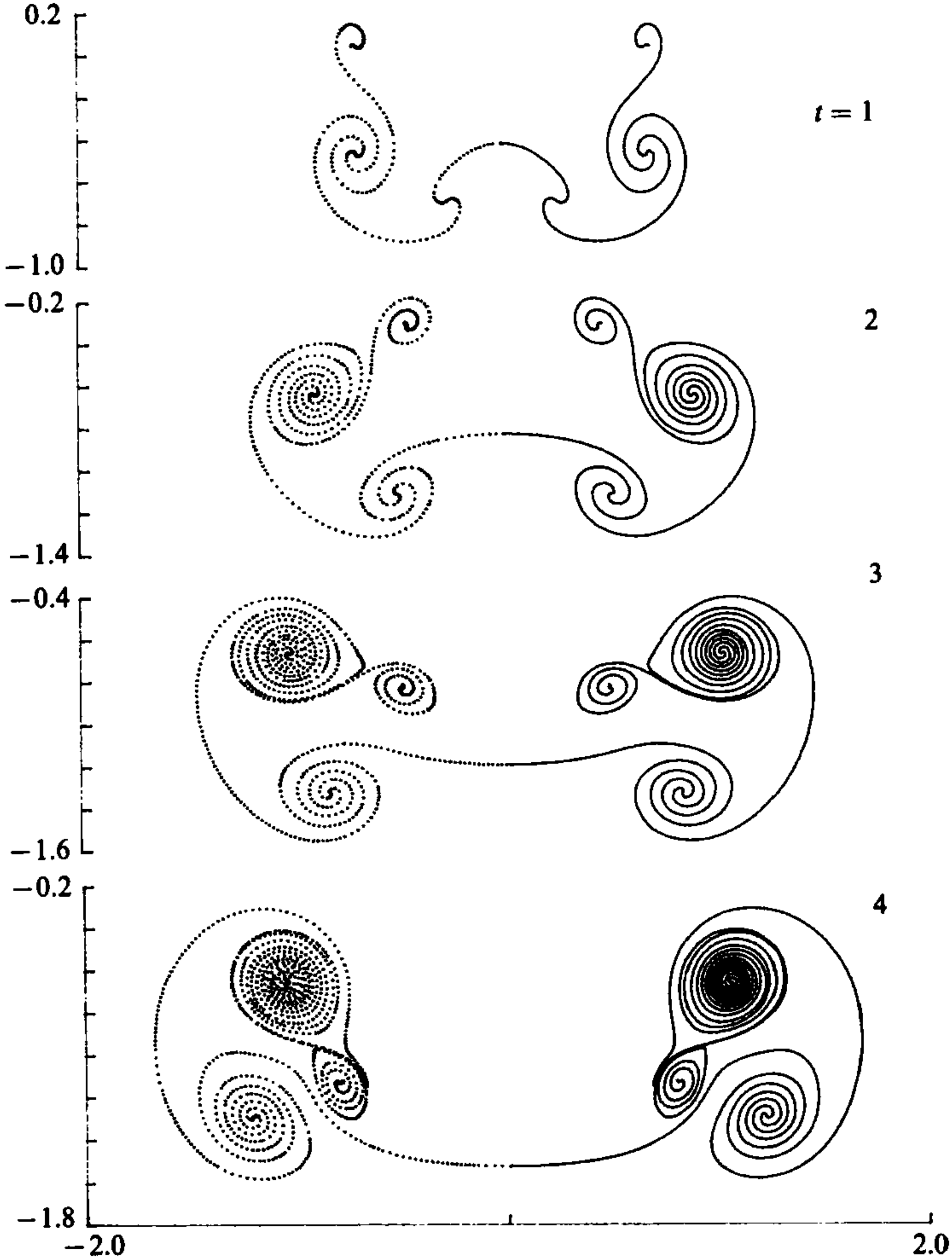


FIG. 154.—Surface of discontinuity behind a wing.

elliptically loaded wing ($N = 200\,, \delta = 0.05$)



fuselage/flap loading



charged particle systems

$x_i \in \mathbb{R}^3$: location , q_i : charge , $i = 1 : N$

$$\phi(x) = \sum_{i=1}^{N} \frac{q_i}{|x - x_i|} \ : \ \text{electric potential} \ , \ -\nabla^2 \phi(x) = \sum_{i=1}^{N} 4\pi q_i \delta(x - x_i)$$

$$V = \frac{1}{2} \sum_{i=1}^{N} q_i \phi_i \ , \ \phi_i = \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{q_j}{|x_i - x_j|} \ : \ \text{potential energy}$$

$$F_i = q_i E_i = -q_i \nabla \phi(x_i) = q_i \sum_{\substack{j=1 \\ j \neq i}}^{N} q_j \frac{x_i - x_j}{|x_i - x_j|^3} \ : \ \text{force on particle } x_i$$

Note that V, F_i can be computed by mesh-based methods, but we will consider mesh-free methods.

direct summation : $O(N^2)$

compute V, F_i by loops over i, j

cutoff method : $O(N)$

$$\phi_i = \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{q_j}{|x_i - x_j|} \approx \sum_{x_j \in B_R(x_i)} \frac{q_j}{|x_i - x_j|} \ , \ B_R(x_i) = \{x : |x - x_i| \leq R\}$$

This works for short-range interactions (e.g. Lennard-Jones), but not for electrostatics since the Coulomb potential decays slowly in space and the cutoff introduces artifacts.

Barnes-Hut treecode : $O(N \log N)$

tree : hierarchical division of the particles into clusters C

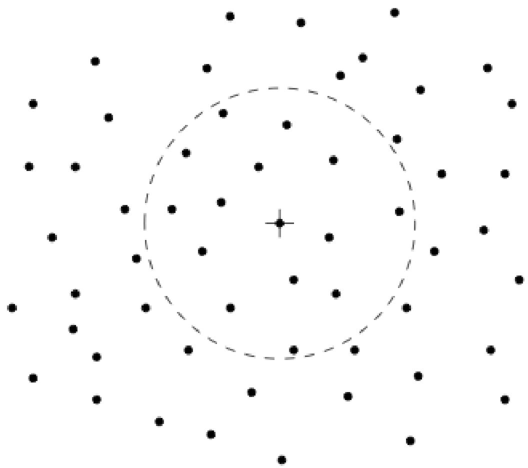
$$\phi_i = \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{q_j}{|x_i - x_j|} = \sum_{C} \sum_{x_j \in C} \frac{q_j}{|x_i - x_j|} \ : \ \text{the choice of clusters depends on } x_i$$

BH computes nearby particle-particle interactions directly and uses a monopole approximation to compute well-separated particle-cluster interactions.

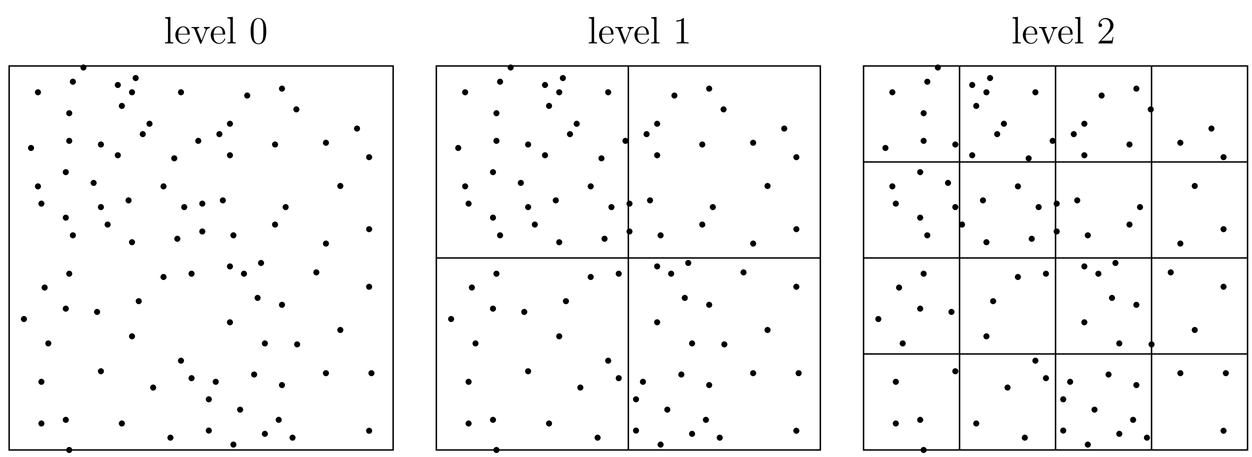
$$\phi_i = \sum_{x_j \in C} \frac{q_j}{|x_i - x_j|} \approx \frac{Q_C}{|x_i - x_c|} \ : \ \text{monopole approximation}$$

$$Q_C = \sum_{x_j \in C} q_j \ : \ \text{total charge in } C \ , \ x_c : \text{cluster center}$$

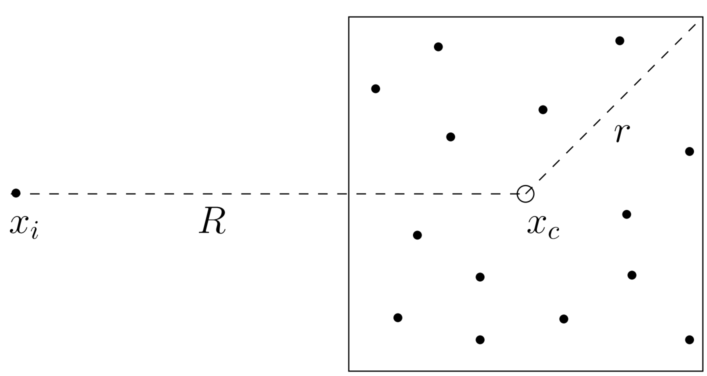
<u>cutoff method</u>



<u>tree structure</u>



<u>particle-cluster interaction</u>

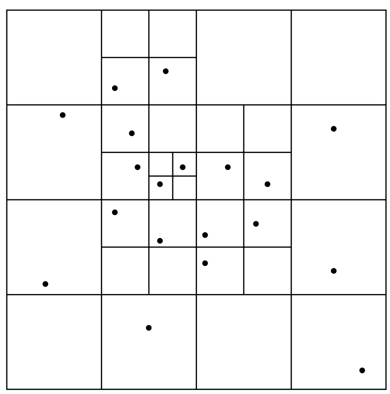


r : cluster radius , R : particle-cluster distance

x_i and C are <u>well-separated</u> $\Leftrightarrow \dfrac{r}{R} \leq \theta$: multipole acceptance criterion (MAC)

<u>program</u> potential_energy
% input : x_i , q_i , $i = 1 : N$
% θ : MAC parameter
% N_0 : maximum number of particles in a leaf of the tree
% output : V
construct tree
for $i = 1 : N$, compute_interaction(x_i , root), end
<u>function</u> compute_interaction(x_i , C)
if $r/R \le \theta$
    compute and store Q_C , x_c (unless done before)
    compute interaction by monopole approximation
else
    if C is a leaf, compute interaction by direct summation
    else, for each child C' of C, compute_interaction(x_i , C')
end

<u>example</u> : $N_0 = 1$



<u>operation count</u> : assume uniform particle density , $N = 8^L$

level 0 : 1 cluster with N particles

level 1 : 8 clusters with $N/8$ particles

level 2 : 8^2 clusters with $N/8^2$ particles

⋮

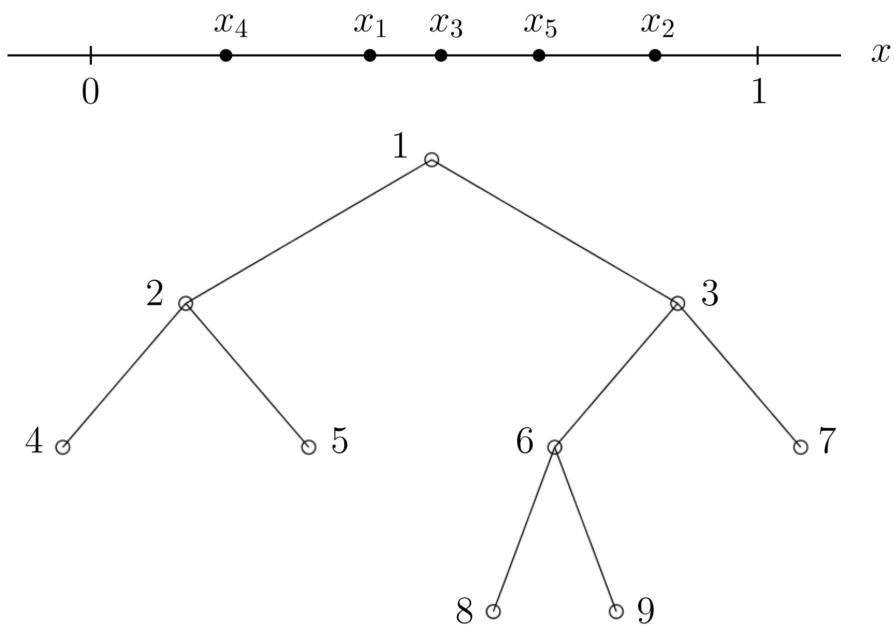
level L : $8^L = N$ clusters with $N/8^L = 1$ particle

There are $L = \log_8 N$ levels in the tree, and each particle does an amount of work at each level that is independent of N, hence BH requires $O(N \log N)$ flops.

1. forces : $F_i = q_i \sum_C \sum_{x_j \in C} q_j \dfrac{x_i - x_j}{|x_i - x_j|^3}$, $\sum_{x_j \in C} q_j \dfrac{x_i - x_j}{|x_i - x_j|^3} \approx Q_C \dfrac{x_i - x_c}{|x_i - x_c|^3}$

2. The monopole approximation is the 1st term in a <u>multipole expansion</u> of the particle-cluster interaction; the accuracy is improved using higher-order terms.

<u>example</u> : $N = 5$, $N_0 = 1$, particles = [0.4186 0.8462 0.5252 0.2026 0.6721]




```
>> tree = m671b_build_tree
tree =
1×9 struct array with fields:
    interval
    members
    children
>> tree(1)
ans =
    interval: [0 1]
    members: [1 2 3 4 5]
    children: [2 3]
>> tree(2)
ans =
    interval: [0 0.5000]
    members: [1 4]
    children: [4 5]
>> tree(3)
ans =
    interval: [0.5000 1]
    members: [2 3 5]
    children: [6 7]
>> tree(4)
ans =
    interval: [0 0.2500]
    members: 4
    children: [ ]
>> tree(5)
ans =
    interval: [0.2500 0.5000]
    members: 1
    children: [ ]
>> tree(6)
ans =
    interval: [0.5000 0.7500]
    members: [3 5]
    children: [8 9]
>> tree(7)
ans =
    interval: [0.7500 1]
    members: 2
    children: [ ]
>> tree(8)
ans =
    interval: [0.5000 0.6250]
    members: 3
    children: [ ]
>> tree(9)
ans =
    interval: [0.6250 0.7500]
    members: 5
    children: [ ]
```

```
function tree_out = m671b_build_tree % Barnes-Hut
global tree particles node_count N0
% N = 100; N0 = 1; rand_N = rand(N,1); particles = rand_N(:,1);
N = 5; N0 = 1; particles = [0.4186 0.8462 0.5252 0.2026 0.6721];
tree = struct( 'interval' , [] , 'members' , [] , 'children' , [] );
tree(1).interval = [0,1];
tree(1).members = 1:N;
node_count = 1;
root = 1; build_tree(root); tree_out = tree;
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function build_tree(cluster_index)
global tree particles node_count N0
child = struct( 'interval' , [] , 'members' , [] , 'children' , [] );
n = length(tree(cluster_index).members);
if (n > N0)
  %
  % step 1 : define intervals for child clusters
  %
  a = tree(cluster_index).interval(1); b = tree(cluster_index).interval(2);
  midpoint = (a+b)/2;
  child(1).interval = [a midpoint]; child(2).interval = [midpoint b];
  %
  % step 2 : insert particles from parent into child clusters
  %
  count(1) = 0; count(2) = 0;
  for j = 1:n
    particle_index = tree(cluster_index).members(j);
    index = 1; if particles(particle_index) > midpoint; index = 2; end
    child(index).members = [child(index).members particle_index];
    count(index) = count(index) + 1;
  end
  %
  % step 3 : add non-empty children to tree
  %
  for j = 1:2
    if (count(j) >= 1)
      node_count = node_count + 1;
      tree(cluster_index).children = [tree(cluster_index).children node_count];
      tree = [tree child(j)];
    end
  end
  %
  % step 4 : recursive call to build next level of children
  %
  for i = 1:length(tree(cluster_index).children)
    cluster_index_new = tree(cluster_index).children(i);
    build_tree(cluster_index_new);
  end
end
```

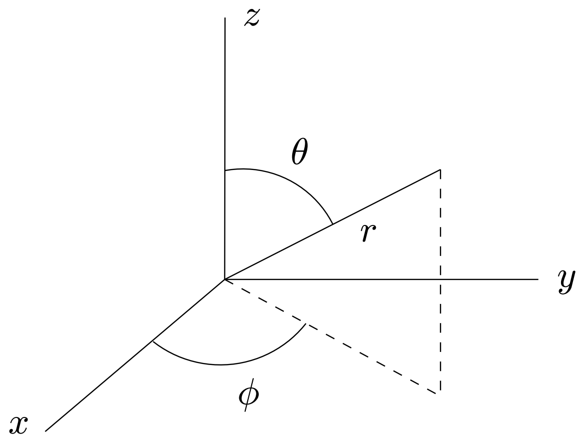
<u>goal</u> : multipole expansion (Folland, Wallace)

Let $x_1, \ldots, x_N \in \mathbb{R}^3$ be a set of point charges.

$$\Phi(x) = \sum_{i=1}^{N} \frac{q_i}{|x - x_i|} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{M_n^m}{r^{n+1}} Y_n^m(\theta, \phi)$$

$Y_n^m(\theta,\phi)$: spherical harmonics , $M_n^m = \sum_{i=1}^{N} q_i \, r_i^n \, Y_n^{-m}(\theta_i, \phi_i)$: moments

$x = (r, \theta, \phi)$, $x_i = (r_i, \theta_i, \phi_i)$: spherical coordinates



$x = r \sin\theta \cos\phi$, $y = r \sin\theta \sin\phi$, $z = r\cos\theta$

$r = \sqrt{x^2 + y^2 + z^2}$, $r \geq 0$

θ : co-latitude , $0 \leq \theta \leq \pi$

ϕ : longitude , $0 \leq \phi \leq 2\pi$

consider $\nabla^2 \Phi = 0$

$$\Phi = \Phi(r,\theta,\phi) \Rightarrow \nabla^2\Phi = \frac{1}{r^2}\big(r^2 \Phi_r\big)_r + \frac{1}{r^2 \sin\theta}\big(\sin\theta\, \Phi_\theta\big)_\theta + \frac{1}{r^2 \sin^2\theta}\Phi_{\phi\phi} = 0$$

separation of variables

multiply by r^2, set $\Phi(r,\theta,\phi) = R(r)S(\theta,\phi)$, divide by RS

$$\frac{1}{R}\big(r^2 R_r\big)_r + \frac{1}{S\sin\theta}\big(\sin\theta\, S_\theta\big)_\theta + \frac{1}{S\sin^2\theta} S_{\phi\phi} = 0$$

$$\Rightarrow \frac{1}{R}\big(r^2 R_r\big)_r = \lambda \; , \; \frac{1}{S\sin\theta}\big(\sin\theta\, S_\theta\big)_\theta + \frac{1}{S\sin^2\theta} S_{\phi\phi} = -\lambda$$

multiply by $\sin^2\theta$, set $S(\theta,\phi) = f(\theta)g(\phi)$

$$\frac{1}{f}\sin\theta\big(\sin\theta\, f_\theta\big)_\theta + \lambda\sin^2\theta + \frac{1}{g}g_{\phi\phi} = 0$$

$$\Rightarrow\ \frac{1}{f}\sin\theta\big(\sin\theta\, f_\theta\big)_\theta + \lambda\sin^2\theta = m^2\ ,\ \ \frac{1}{g}g_{\phi\phi} = -m^2$$

$g_{\phi\phi} + m^2 g = 0$ + PBC $\Rightarrow\ g(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi}\,,\ m = 0,\ \pm1,\ \pm2,\ \ldots$: Fourier series

$$f_{\theta\theta} + \frac{\cos\theta}{\sin\theta}f_\theta + \left(\lambda - \frac{m^2}{\sin^2\theta}\right)f = 0$$: e-value problem

claim : The equation for f has regular singular points at $\theta = 0\,,\pi$ (more later); there are no explicit BCs; instead, the e-function f is required to have a finite limit at $\theta = 0,\pi$; for each integer m, there is an infinite sequence of e-values λ; the corresponding e-spaces are 1-dimensional and mutually orthogonal.

special case : $m = 0$, we will verify these claims in this case

Then $\Phi(r,\theta,\phi)$ is independent of ϕ and hence is axisymmetric about z-axis.

$$f_{\theta\theta} + \frac{\cos\theta}{\sin\theta}f_\theta + \lambda f = 0$$

set $s = \cos\theta\,,\ -1 \le s \le 1\,,\ f(\theta) = F(s)$

$$f_\theta = F_s s_\theta = F_s \cdot -\sin\theta = -\sin\theta F_s$$

$$f_{\theta\theta} = -\sin\theta F_{ss}\cdot -\sin\theta - \cos\theta F_s = \sin^2\theta F_{ss} - \cos\theta F_s$$

$$\Rightarrow\ \sin^2\theta F_{ss} - \cos\theta F_s + \frac{\cos\theta}{\sin\theta}\cdot -\sin\theta F_s + \lambda F = 0$$

$\Rightarrow\ (1-s^2)F_{ss} - 2sF_s + \lambda F = 0$: Legendre equation

$\Rightarrow\ ((1-s^2)F_s)_s + \lambda F = 0$: Sturm-Liouville form

The Legendre equation has regular singular points at $s = \pm1$. (more later)

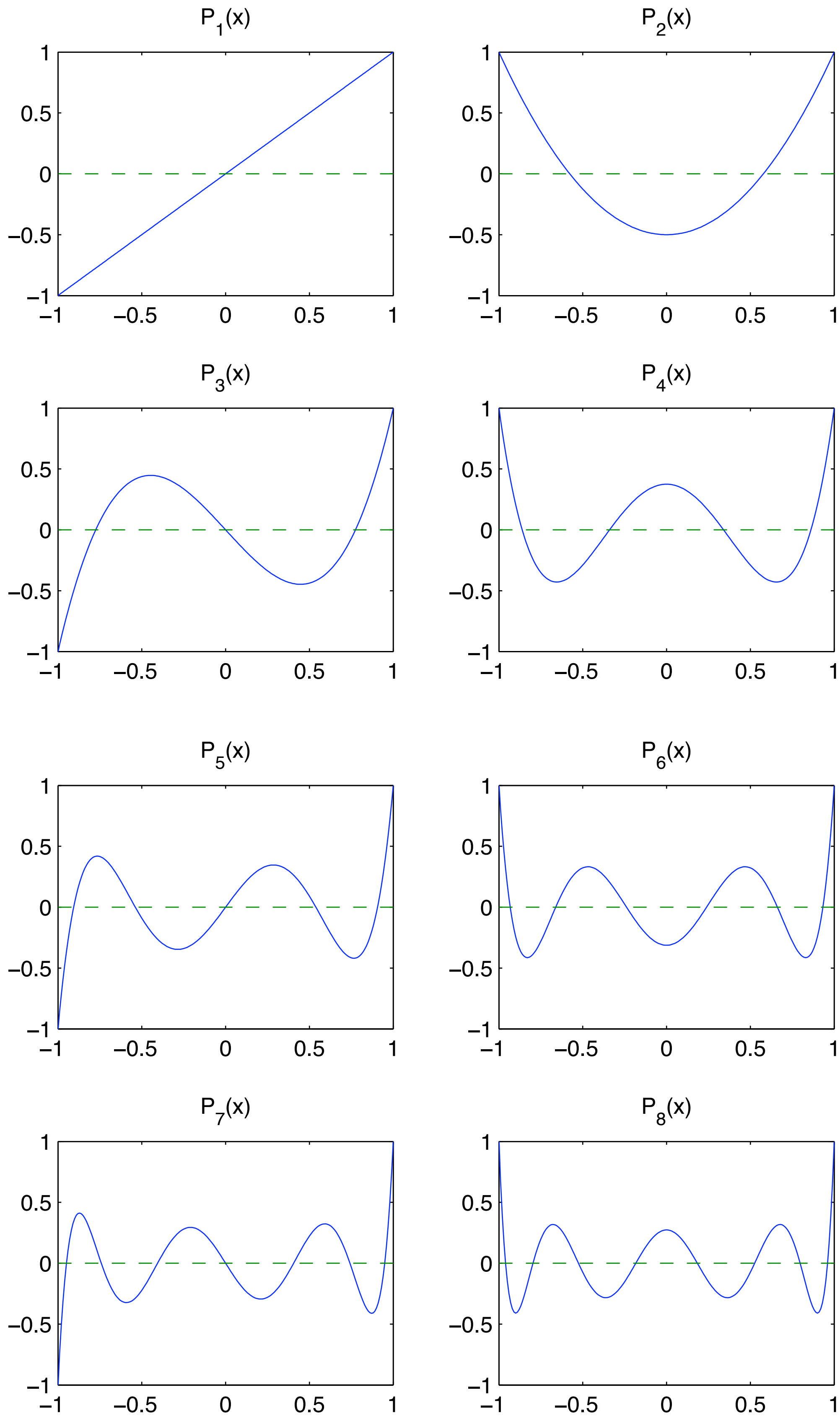
def : $P_n(x) = \dfrac{1}{2^n n!}\dfrac{d^n}{dx^n}(x^2-1)^n$: Rodrigues formula

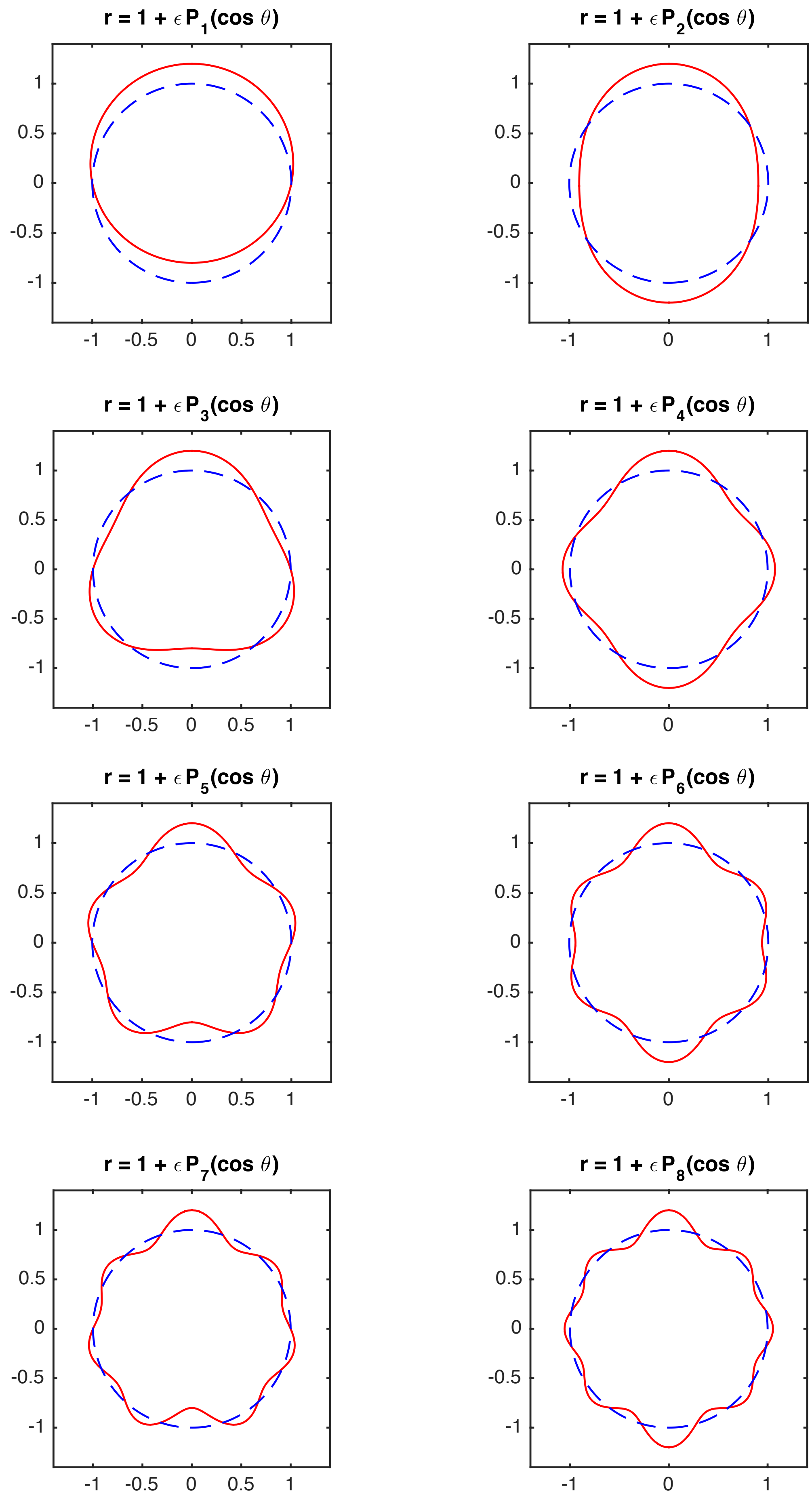
$P_n(x)$ is the Legendre polynomial of degree n

$$P_0(x) = 1$$

$$P_1(x) = \tfrac{1}{2}\tfrac{d}{dx}(x^2-1) = \tfrac{1}{2}(2x) = x$$

$$P_2(x) = \tfrac{1}{4\cdot 2}\tfrac{d^2}{dx^2}(x^2-1)^2 = \tfrac{1}{8}\tfrac{d^2}{dx^2}(x^4-2x^2+1) = \tfrac{1}{8}(12x^2-4) = \tfrac{3}{2}x^2 - \tfrac{1}{2}$$


P1(x)
P2(x)
P3(x)
P4(x)
P5(x)
P6(x)
P7(x)
P8(x)



$r = 1 + \epsilon P_1(\cos\theta)$
$r = 1 + \epsilon P_2(\cos\theta)$
$r = 1 + \epsilon P_3(\cos\theta)$
$r = 1 + \epsilon P_4(\cos\theta)$
$r = 1 + \epsilon P_5(\cos\theta)$
$r = 1 + \epsilon P_6(\cos\theta)$
$r = 1 + \epsilon P_7(\cos\theta)$
$r = 1 + \epsilon P_8(\cos\theta)$

<u>properties of Legendre polynomials</u>

1. $((1-x^2)P_n'(x))' + n(n+1)P_n(x) = 0$: Legendre equation , $\lambda = n(n+1)$

2. $\int_{-1}^{1} P_n(x)P_m(x)dx = 0$ if $n \neq m$: orthogonality

<u>pf</u>

1. $n = 0, 1$: ok , consider $n \geq 2$

set $y = (x^2-1)^n \Rightarrow y' = n(x^2-1)^{n-1} \cdot 2x \Rightarrow (x^2-1)y' = 2nxy$

differentiate both sides $n+1$ times

recall : $(fg)^{(n)} = fg^{(n)} + nf^{(1)}g^{(n-1)} + \frac{1}{2}n(n-1)f^{(2)}g^{(n-2)} + \cdots$

$$(x^2-1)y^{(n+2)} + (\cancel{n}+1)2xy^{(n+1)} + \tfrac{1}{2}(n+1)n2y^{(n)} = 2n(\cancel{xy^{(n+1)}} + (n+1)y^{(n)})$$

$$\Rightarrow (x^2-1)y^{(n+2)} + 2xy^{(n+1)} - n(n+1)y^{(n)} = 0$$

$$\Rightarrow (1-x^2)y^{(n+2)} - 2xy^{(n+1)} + n(n+1)y^{(n)} = 0$$

note : $y^{(n)} = \dfrac{d^n}{dx^n}(x^2-1)^n = 2^n n! P_n(x)$

$\Rightarrow (1-x^2)P_n''(x) - 2xP_n'(x) + n(n+1)P_n(x) = 0$ <u>ok</u>

2. $((1-x^2)P_n'(x))' + n(n+1)P_n(x) = 0$

$$\Rightarrow \int_{-1}^{1} \left[((1-x^2)P_n'(x))'P_m(x) + n(n+1)P_n(x)P_m(x)\right] dx = 0$$

note : $(1-x^2)P_n'(x)P_m(x)\Big|_{-1}^{1} = 0$

$$\Rightarrow -\int_{-1}^{1}(1-x^2)P_n'(x)P_m'(x)dx + n(n+1)\int_{-1}^{1}P_n(x)P_m(x)dx = 0$$

switch m and n

$$\Rightarrow -\int_{-1}^{1}(1-x^2)P_m'(x)P_n'(x)dx + m(m+1)\int_{-1}^{1}P_m(x)P_n(x)dx = 0$$

subtract $\Rightarrow ((n(n+1) - m(m+1))\int_{-1}^{1}P_n(x)P_m(x)dx = 0$ <u>ok</u>

Hence the Legendre equation has e-values $\lambda = n(n+1)$ for $n = 0, 1, 2, \ldots,$ and the corresponding e-functions $P_n(x)$ form an orthogonal basis for $L^2(-1,1)$.

pf : completeness . . .

note : this is analogous to the spectral factorization of a real symmetric matrix background : series solutions of differential equations

def : A function $y(x)$ is analytic at x_0 if it has a convergent power series expansion in a neighborhood of x_0, i.e. $y(x) = \sum\limits_{k=0}^{\infty} b_k(x-x_0)^k$ for $|x-x_0| < R$, where $R > 0$; in this case $b_k = y^{(k)}(x_0)/k!$; otherwise $y(x)$ is singular at x_0.

Consider $y'' + a_1(x)y' + a_2(x)y = 0$: 2nd order, linear, variable coefficient ODE.

question : are the solutions $y(x)$ analytic or singular at a given x_0?

thm : classification of x_0

1. ordinary point : $a_1(x)$ and $a_2(x)$ are analytic at x_0

$\Rightarrow$ given $y(x_0), y'(x_0)$, we can solve for $y''(x_0), y'''(x_0), \ldots$

$\Rightarrow$ there are two linearly independent analytic solutions at x_0

example : $y'' + y = 0 \Rightarrow a_1(x) = 0\,,\ a_2(x) = 1$: all points x_0 are ordinary

$$y(x) = c_1 \sin x + c_2 \cos x$$

2. singular point : $a_1(x)$ or $a_2(x)$ is singular at x_0

2a. regular singular point : $(x-x_0)a_1(x)$ and $(x-x_0)^2 a_2(x)$ are analytic at x_0, i.e. $y'' + \dfrac{\tilde{a}_1(x)}{x-x_0}\,y' + \dfrac{\tilde{a}_2(x)}{(x-x_0)^2}\,y = 0$, where $\tilde{a}_1(x), \tilde{a}_2(x)$ are analytic at x_0; in this case we cannot directly solve for $y''(x_0), y'''(x_0), \ldots$; nonetheless, there is at least one solution of the form $y(x) = \sum\limits_{k=0}^{\infty} b_k(x-x_0)^{k+s}$ for some $s \in \mathbb{R}$, and $y(x)$ is analytic at $x_0 \Leftrightarrow s \in \{0, 1, 2, \ldots\}$

example : $x^2 y'' + \dfrac{1}{4}y = 0 \Rightarrow y'' + \dfrac{1}{4x^2}y = 0$: regular singular point at $x_0 = 0$

$$y(x) = c_1 x^{1/2} + c_2 x^{1/2} \ln x \ , \text{ check } \ldots$$

example : $(1-x^2)y'' - 2xy' = 0$: Legendre equation , $n = 0$

$$y'' - \frac{2x}{1-x^2}\,y' = 0 : \text{ regular singular points at } x_0 = \pm 1$$

$$y(x) = c_1 + c_2 \ln \frac{1+x}{1-x} \ , \text{ check } \ldots$$

2b. irregular singular point : x_0 is singular point, but not regular singular point

$\Rightarrow$ an analytic solution at x_0 may or may not exist

example : $x^4 y'' + 2x^3 y' + y = 0$

$$y'' + \frac{2}{x}\,y' + \frac{1}{x^4}\,y = 0 : \text{ irregular singular point at } x_0 = 0$$

$$y(x) = c_1 \sin\frac{1}{x} + c_2 \cos\frac{1}{x}\ \text{, check} \ldots \text{, no solution is analytic at } x_0 = 0$$

<u>example</u> : $(1-x^2)y''-2xy'+n(n+1)y = 0$: Legendre equation , $n = 0, 1, 2, \ldots$

$x_0 = 0$ is an ordinary point , we will verify the theorem

$y = \sum_{k=0}^{\infty} b_k x^k$, $y' = \sum_{k=0}^{\infty} b_k k x^{k-1}$, $y'' = \sum_{k=0}^{\infty} b_k k(k-1)x^{k-2}$

$\sum_{k=0}^{\infty} b_k k(k-1)x^{k-2} - \sum_{k=0}^{\infty} b_k k(k-1)x^k - 2\sum_{k=0}^{\infty} b_k k x^k + n(n+1)\sum_{k=0}^{\infty} b_k x^k = 0$

$\Rightarrow \sum_{k=0}^{\infty} b_k k(k-1)x^{k-2} - \sum_{k=0}^{\infty} b_k(k(k-1)+2k-n(n+1))x^k = 0$

set $f_k = k(k-1)$, so $k(k-1)+2k = k(k+1) = f_{k+1}$

$\Rightarrow \sum_{k=0}^{\infty} b_k f_k x^{k-2} - \sum_{k=0}^{\infty} b_k(f_{k+1}-f_{n+1})x^k = 0$

$\Rightarrow \sum_{k=0}^{\infty} b_k f_k x^{k-2} - \sum_{k=2}^{\infty} b_{k-2}(f_{k-1}-f_{n+1})x^{k-2} = 0$

note : $b_0 f_0 x^{-2} + b_1 f_1 x^{-1} = 0$ because $f_0 = f_1 = 0$

$\Rightarrow \sum_{k=2}^{\infty} (b_k f_k - b_{k-2}(f_{k-1}-f_{n+1}))x^{k-2} = 0$

$\Rightarrow b_k f_k = b_{k-2}(f_{k-1}-f_{n+1})$ for $k \geq 2$

<u>case 1</u> : $b_0 \neq 0$, $b_1 = 0$

$\Rightarrow b_3 = b_5 = b_7 = \cdots = 0 \Rightarrow$ we may assume k is even

<u>case 1a</u> : n is even $\Rightarrow f_{k-1} = f_{n+1}$ for $k = n+2 \Rightarrow b_k = 0$ for $k \geq n+2$

$\Rightarrow y(x)$ is an even polynomial of degree n , $P_n(x)$

<u>case 1b</u> : n is odd $\Rightarrow f_{k-1} \neq f_{n+1}$ for $k \geq 2$

$\Rightarrow y(x)$ is an even non-terminating power series : $Q_n(x)$, convergence ...

<u>case 2</u> : $b_0 = 0$, $b_1 \neq 0$

$\Rightarrow b_2 = b_4 = b_6 = \cdots = 0 \Rightarrow$ we may assume k is odd , ... $\begin{cases} n : \text{even} \Rightarrow Q_n(x) \\ n : \text{odd} \Rightarrow P_n(x) \end{cases}$

<u>general solution</u> : $y(x) = c_1 P_n(x) + c_2 Q_n(x)$

recall : A previous example showed that $Q_0(x) = \ln\frac{1+x}{1-x}$, which is analytic at $x = 0$, but singular at $x = \pm 1$; in fact, $Q_n(x)$ is singular at $x = \pm 1$ for all $n \geq 0$.

more properties of Legendre polynomials

1. $\displaystyle\sum_{n=0}^{\infty} P_n(x)t^n = \frac{1}{\sqrt{1-2xt+t^2}}$: generating function , holds for $|x| \leq 1\,, |t| < 1$

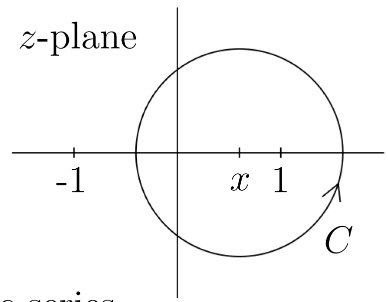
note : $1 - 2xt + t^2 = t^2 - 2xt + x^2 - x^2 + 1 = (t-x)^2 + 1 - x^2 \geq 0$

note : $x = 1 \Rightarrow \displaystyle\sum_{n=0}^{\infty} P_n(1)t^n = \frac{1}{\sqrt{1-2t+t^2}} = \frac{1}{1-t} = \sum_{n=0}^{\infty} t^n \Rightarrow P_n(1) = 1$

2. $\displaystyle||P_n||^2 = \int_{-1}^{1} P_n(x)^2 dx = \frac{2}{2n+1}$

3. $(n+1)P_{n+1}(x) - (2n+1)xP_n(x) + nP_{n-1}(x) = 0$: recurrence relation , $n \geq 1$

pf : 1. recall : $\displaystyle\frac{1}{2\pi i}\int_C \frac{f(z)}{(z-z_0)^{n+1}}\,dz = \frac{f^{(n)}(z_0)}{n!}$: Cauchy integral formula



set $f(z) = \dfrac{(z^2-1)^n}{2^n}$, $z_0 = x$, $C = \{z : |z - x| = 1\}$

$$\frac{1}{2\pi i}\int_C \frac{(z^2-1)^n}{2^n(z-x)^{n+1}}\,dz = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n = P_n(x)$$

$$\sum_{n=0}^{\infty} P_n(x)t^n = \frac{1}{2\pi i}\int_C \sum_{n=0}^{\infty}\left(\frac{t}{2}\right)^n \frac{(z^2-1)^n}{(z-x)^{n+1}}\,dz : \begin{cases}\text{geometric series,} \\ \text{converges uniformly} \\ \text{for small } t \text{ and } z \in C\end{cases}$$

$$= \frac{1}{2\pi i}\int_C \frac{1}{z-x}\left(1 - \frac{t(z^2-1)}{2(z-x)}\right)^{-1} dz$$

$$= \frac{1}{2\pi i}\int_C \frac{2}{2(z-x) - t(z^2-1)}\,dz \ : \text{ evaluate by residue theorem}$$

$$-tz^2 + 2z + t - 2x = 0 \Rightarrow z = \frac{-2 \pm \sqrt{4 - 4(-t)(t-2x)}}{-2t} = \frac{1 \pm \sqrt{1-2xt+t^2}}{t}$$

$z_1 = \dfrac{1 - \sqrt{1-2xt+t^2}}{t}$, $\displaystyle\lim_{t\to 0} z_1 = x \Rightarrow z_1$ is inside C , z_2 is outside C

$$\sum_{n=0}^{\infty} P_n(x)t^n = \text{Res}\left(\frac{2}{-t(z-z_1)(z-z_2)}\,; z = z_1\right) = \frac{2}{-t(z_1-z_2)} = \frac{1}{\sqrt{1-2xt+t^2}}$$

This proves the result for small t, but the series is the Taylor series of a function which is analytic at $t = 0$ and whose only singularities are at $t = x \pm i\sqrt{1-x^2}$, which satisfy $|t| = 1$, so the series converges for $|t| < 1$. ok

2. square and integrate

$$\int_{-1}^{1} \frac{dx}{1-2xt+t^2} = \int_{-1}^{1}\left(\sum_{n=0}^{\infty} P_n(x)t^n\right)^2 dx = \sum_{n=0}^{\infty}\int_{-1}^{1} P_n(x)^2 dx \cdot t^{2n}$$

$$= \left.\frac{\ln(1-2xt+t^2)}{-2t}\right|_{-1}^{1} = -\frac{1}{2t}\ln\left(\frac{1-2t+t^2}{1+2t+t^2}\right) = \frac{1}{t}\ln\frac{1+t}{1-t}$$

$$\frac{1}{1+t} = \sum_{l=0}^{\infty}(-t)^n \Rightarrow \ln(1+t) = \sum_{n=0}^{\infty}\frac{(-1)^n t^{n+1}}{n+1}$$

$$\frac{1}{1-t} = \sum_{n=0}^{\infty} t^n \Rightarrow -\ln(1-t) = \sum_{n=0}^{\infty}\frac{t^{n+1}}{n+1}$$

$$\Rightarrow \frac{1}{t}\ln\frac{1+t}{1-t} = \sum_{n=0}^{\infty}\frac{2}{2n+1}t^{2n} \quad \underline{\text{ok}}$$

3. set $f(t) = (1-2xt+t^2)^{-1/2}$, then $P_n(x) = \dfrac{f^{(n)}(0)}{n!}$

$f'(t) = -\frac{1}{2}(1-2xt+t^2)^{-3/2}\cdot(-2x+2t) \Rightarrow (1-2xt+t^2)f'(t) = (x-t)f(t)$

differentiate n times wrt t

$$(1-2xt+t^2)f^{(n+1)}(t) + n(-2x+2t)f^{(n)}(t) + \tfrac{1}{2}n(n-1)2f^{(n-1)}(t)$$
$$= (x-t)f^{(n)}(t) + n(-1)f^{(n-1)}(t)$$

set $t=0$: $f^{(n+1)}(0) - 2nxf^{(n)}(0) + n(n-1)f^{(n-1)}(0) = xf^{(n)}(0) - nf^{(n-1)}(0)$

divide by $(n+1)!$: $\dfrac{f^{(n+1)}(0)}{(n+1)!} - \dfrac{(2n+1)xf^{(n)}(0)}{(n+1)!} + \dfrac{n^2 f^{(n-1)}(0)}{(n+1)!} = 0$ <u>ok</u>

<u>check</u>

1. generating function

recall : $(1+x)^k = 1 + kx + \frac{1}{2}k(k-1)x^2 + \cdots$

set $k = -\frac{1}{2}$, $x \to -2xt+t^2$

$(1-2xt+t^2)^{-1/2} = 1 - \frac{1}{2}(-2xt+t^2) + \frac{1}{2}(-\frac{1}{2})(-\frac{3}{2})(-2xt+t^2)^2 + \cdots$

match coeffs of t^n : $P_0(x) = 1$, $P_1(x) = x$, $P_2(x) = -\frac{1}{2} + \frac{3}{8}\cdot 4x^2 = \frac{3}{2}x^2 - \frac{1}{2}$

2. recurrence relation

$n = 1 \Rightarrow 2P_2(x) - 3xP_1(x) + P_0(x) = 0 \Rightarrow P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}$

hw4 : derive $P_3(x)$, $P_4(x)$

recall : $\dfrac{1}{R}\big(r^2 R_r\big)_r = \lambda = n(n+1)$, radial equation

$r^2 R_{rr} + 2rR_r - n(n+1)R = 0$

$a_1(r) = \dfrac{2}{r}$, $a_2(r) = -\dfrac{n(n+1)}{r^2}$: regular singular point at $r = 0$

$$R(r) = r^s \ \Rightarrow\ s(s-1)r^s + 2sr^s - n(n+1)r^s = 0$$
$$\Rightarrow\ s^2 + s - n(n+1) = (s-n)(s+(n+1)) = 0 \ \Rightarrow\ s = n\,, -(n+1)$$
$$\Rightarrow\ R(r) = ar^n + \frac{b}{r^{n+1}}$$

general axisymmetric solution of $\nabla^2\Phi = 0$

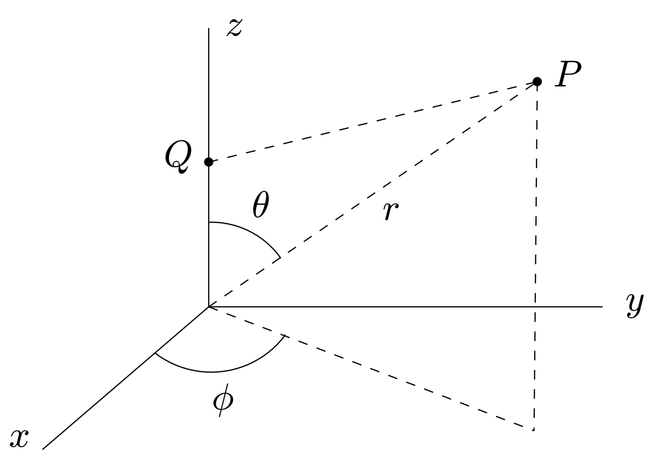
$$\Phi(r,\theta,\phi) = \sum_{n=0}^{\infty}\Big(a_n r^n + \frac{b_n}{r^{n+1}}\Big)P_n(\cos\theta)\ :\ \text{axisymmetric wrt } z\text{-axis}$$

A singularity is allowed at $r = 0$, but not at $\theta = 0, \pi$.

example 1 : potential due to a point charge at the origin

$$\Phi(r,\theta,\phi) = \frac{1}{r}\ ,\ -\nabla^2\Big(\frac{1}{r}\Big) = 4\pi\delta(r)\ :\ \text{hw3}$$

example 2 : potential at P due to a point charge at Q on the z-axis



$$Q = (0,0,z_0)$$
$$P = (x,y,z)$$
$$= (r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta)$$

$$\Phi(r,\theta,\phi) = \frac{1}{|P-Q|} = \frac{1}{\sqrt{x^2+y^2+(z-z_0)^2}} = \frac{1}{\sqrt{r^2 - 2(r\cos\theta)z_0 + z_0^2}}$$

Since Φ is axisymmetric, it can be expressed in the general form above.

$$|z_0| < r \Rightarrow \Phi(r,\theta,\phi) = \frac{1}{r}\,\frac{1}{\sqrt{1 - 2\cos\theta(z_0/r) + (z_0/r)^2}} = \sum_{n=0}^{\infty}\frac{z_0^n}{r^{n+1}}P_n(\cos\theta)$$

note : if $z_0 \to 0$, then example 2 $\to$ example 1

$$|z_0| > r\ \Rightarrow\ \Phi(r,\theta,\phi) = \frac{1}{z_0}\,\frac{1}{\sqrt{1 - 2\cos\theta(r/z_0) + (r/z_0)^2}} = \sum_{n=0}^{\infty}\frac{r^n}{z_0^{n+1}}P_n(\cos\theta)$$

<u>alternative viewpoint</u>

$$\Phi(x,y,z;z_0) = \frac{1}{\sqrt{x^2+y^2+(z-z_0)^2}} \ : \ \text{Taylor expand wrt } z_0 \text{ about } z_0 = 0$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \partial_{z_0}^n \Phi\Big|_{z_0=0} z_0^n \ , \ \text{note : } \partial_{z_0}\Phi\Big|_{z_0=0} = -\partial_z \Phi\Big|_{z_0=0} = -\partial_z(r^{-1})$$

$$= \sum_{n=0}^{\infty} z_0^n \frac{(-1)^n}{n!} \partial_z^n (r^{-1}) = \sum_{n=0}^{\infty} M_n(z_0)\Phi_n(x,y,z;0) \ : \ \begin{cases} \text{multipole expansion,} \\ \text{converges for } |z_0| < r \end{cases}$$

$M_n(z_0) = z_0^n$: multipole moments

$$\Phi_n(x,y,z;0) = \frac{(-1)^n}{n!}\partial_z^n(r^{-1}) = \frac{P_n(\cos\theta)}{r^{n+1}} \ : \ \text{multipole potentials}$$

note : This is another way to define the Legendre polynomials.

question : why multipole?

$$\Phi_0(x,y,z;0) = r^{-1} = \frac{P_0(\cos\theta)}{r} \, , \, -\nabla^2\Phi_0 = -\nabla^2(r^{-1}) = 4\pi\delta \ : \ \text{monopole}$$

$$\Phi_1(x,y,z;0) = -\,\partial_z(r^{-1}) = \frac{z}{r^3} = \frac{P_1(\cos\theta)}{r^2}$$

$$-\nabla^2\Phi_1 = -\nabla^2(-\partial_z(r^{-1})) = -\partial_z(-\nabla^2(r^{-1})) = -\,4\pi\partial_z\delta \ : \ \text{dipole}$$

$$\text{note : } -\partial_z\delta(x,y,z;0) = \partial_{z_0}(x,y,z;0) = \lim_{\epsilon\to 0}\left(\frac{\delta(x,y,z;\epsilon)-\delta(x,y,z;-\epsilon)}{2\epsilon}\right)$$

$$\Phi_2(x,y,z;0) = \frac{1}{2}\,\partial_z^2(r^{-1}) = \frac{1}{2}\,\partial_z\left(-\,\frac{z}{r^3}\right) = \frac{1}{2}\cdot -\left(\frac{r^3 - z\cdot 3r^2\cdot z/r}{r^6}\right)$$

$$= \frac{3z^2-r^2}{2r^5} = \frac{P_2(\cos\theta)}{r^3}$$

$$-\nabla^2\Phi_2 = -\nabla^2\left(\frac{1}{2}\partial_z^2(r^{-1})\right) = \frac{1}{2}\partial_z^2(-\nabla^2(r^{-1})) = 2\pi\partial_z^2\delta \ : \ \text{quadrupole}$$

$\Phi_n(x,y,z;0)$: multipole potential of order 2^n along the z-axis at $z_0 = 0$

Hence a monopole charge at $(0,0,z_0)$ and a series of multipole charges at $(0,0,0)$ with moments $M_n(z_0)$ induce the same potential $\Phi(x,y,z;z_0)$ for $r > |z_0|$.

recall : separation of variables for $-\nabla^2\Phi(r,\theta,\phi) = 0\,,\ \dots\,,\ S(\theta,\phi) = f(\theta)g(\phi)$

$g(\phi) = \dfrac{1}{\sqrt{2\pi}}\, e^{im\phi}\ ,\ m = 0,\ \pm 1,\ \pm 2,\ \dots$

$f_{\theta\theta} + \dfrac{\cos\theta}{\sin\theta} f_\theta + \Big(\lambda - \dfrac{m^2}{\sin^2\theta}\Big) f = 0$, set $s = \cos\theta\,,\ f(\theta) = F(s)$

$((1-s^2)F_s)_s + \Big(\lambda - \dfrac{m^2}{1-s^2}\Big) F = 0$: associated Legendre equation

note : regular singular points at $s = \pm 1$

special case : $m = 0 \Rightarrow ((1-s^2)F_s)_s + \lambda F = 0$: Legendre equation

$\lambda = n(n+1)\,,\ F(s) = P_n(s)\,,\ n = 0, 1, 2, \dots$

---

now consider $m = 1, 2, \dots$

claim: If $w(s)$ satisfies LE, then $F(s) = (1-s^2)^{m/2} w^{(m)}(s)$ satisfies ALE.

pf : given $((1-s^2)w_s)_s + \lambda w = 0$, differentiate m times

$\Rightarrow\ ((1-s^2)w_s)^{(m+1)} + \lambda w^{(m)} = 0$

$\Rightarrow\ (1-s^2)w^{(m+2)} + (m+1)(-2s)w^{(m+1)} + \frac{1}{2}(m+1)m(-2)w^{(m)} + \lambda w^{(m)} = 0$

set $F(s) = (1-s^2)^{m/2} w^{(m)}(s)$

$\Rightarrow\ F_s = (1-s^2)^{m/2} w^{(m+1)} + \frac{m}{2}(1-s^2)^{(m/2)-1}(-2s)w^{(m)}$

$\Rightarrow\ (1-s^2)F_s = (1-s^2)^{(m/2)+1} w^{(m+1)} - ms(1-s^2)^{m/2} w^{(m)}$

$\Rightarrow\ ((1-s^2)F_s)_s = (1-s^2)^{(m/2)+1} w^{(m+2)} + (\frac{m}{2}+1)(1-s^2)^{m/2}(-2s)w^{(m+1)}$

$\qquad -ms(1-s^2)^{m/2} w^{(m+1)} - ms\frac{m}{2}(1-s^2)^{(m/2)-1}(-2s)w^{(m)} - m(1-s^2)^{m/2} w^{(m)}$

$\quad = (1-s^2)^{m/2}\left((1-s^2)w^{(m+2)} - 2(m+1)sw^{(m+1)} + (\frac{m^2s^2}{1-s^2} - m)w^{(m)}\right)$

$\quad = (1-s^2)^{m/2}\left((m+1)mw^{(m)} - \lambda w^{(m)} + (\frac{m^2s^2}{1-s^2} - m)w^{(m)}\right)$

$\quad = (m^2(1 + \frac{s^2}{1-s^2}) - \lambda)F = (\frac{m^2}{1-s^2} - \lambda)F$ ok

Now let $\lambda = n(n+1)\,, w(s) = P_n(s)$.

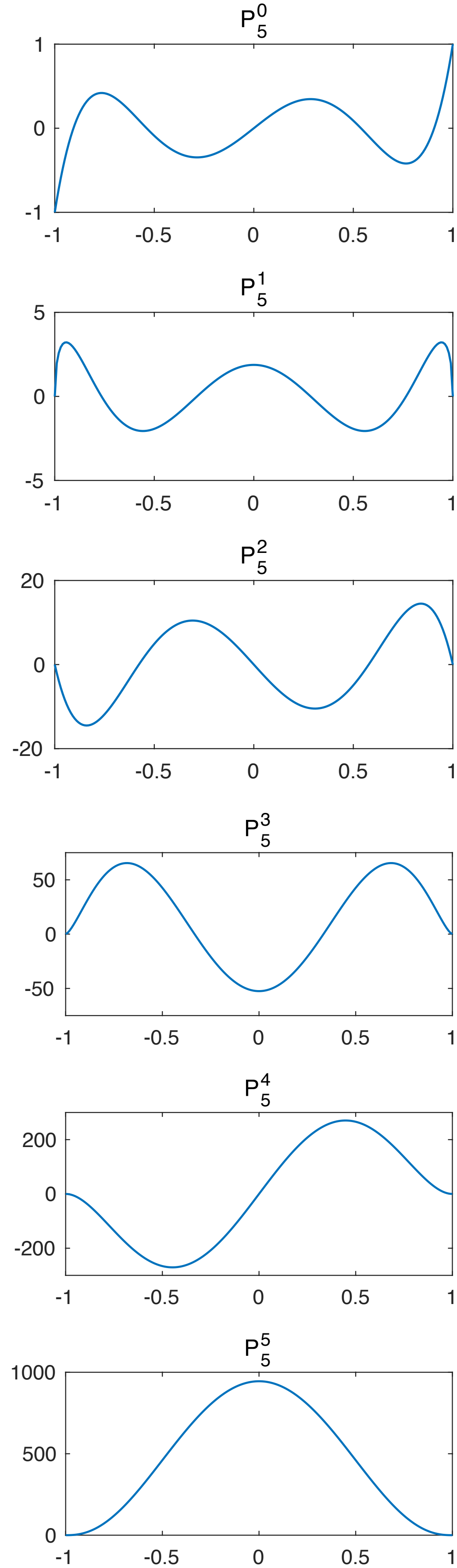
def : $P_n^m(s) = (1-s^2)^{m/2} \dfrac{d^m}{ds^m} P_n(s)$: associated Legendre function , $m = 0 : n$

<u>associated Legendre functions</u>

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n\,,\ n = 0, 1, 2, \ldots$$

$$P_n^m(x) = (1-x^2)^{m/2}\frac{d^m}{dx^m}P_n(x)\,,\ m = 0 : n$$

n	P_n^0
0	1
1	x
2	$\frac{1}{2}(3x^2-1)$
3	$\frac{1}{2}(5x^3-3x)$
4	$\frac{1}{8}(35x^4-30x^2+3)$
5	$\frac{1}{8}(63x^5-70x^3+15x)$
n	P_n^1
1	$(1-x^2)^{1/2}$
2	$3x(1-x^2)^{1/2}$
3	$\frac{3}{2}(5x^2-1)(1-x^2)^{1/2}$
4	$\frac{5}{2}(7x^3-3x)(1-x^2)^{1/2}$
5	$\frac{15}{8}(21x^4-14x^2+1)(1-x^2)^{1/2}$
n	P_n^2
2	$3(1-x^2)$
3	$15x(1-x^2)$
4	$\frac{15}{2}(7x^2-1)(1-x^2)$
5	$\frac{105}{2}(3x^3-x)(1-x^2)$
n	P_n^3
3	$15(1-x^2)^{3/2}$
4	$105x(1-x^2)^{3/2}$
5	$\frac{105}{2}(9x^2-1)(1-x^2)^{3/2}$
n	P_n^4
4	$105(1-x^2)^2$
5	$945x(1-x^2)^2$
n	P_n^5
5	$945(1-x^2)^{5/2}$



<u>claim</u> : For each $m = 0, 1, 2, \ldots$, $\{P_n^m(s)\}_{n=m}^{\infty}$ is an orthogonal basis for $L^2(-1,1)$.

	$n=1$	$n=1$	$n=2$	$n=3$	$\cdots$
$m=0$	P_0^0	P_1^0	P_2^0	P_3^0	$\cdots$
$m=1$		P_1^1	P_2^1	P_3^1	$\cdots$
$m=2$			P_2^2	P_3^2	$\cdots$
$m=3$				P_3^3	$\cdots$
$\vdots$					$\cdots$

note : $\{P_n^m(s)\}_{n=m}^{\infty} = \{P_{m+k}^m(s)\}_{k=0}^{\infty}$

note : $L_w^2(-1,1)$ is a Hilbert space with $<f,g> = \displaystyle\int_{-1}^{1} f(s)g(s)w(s)ds$

<u>pf</u> : the case $m=0$ is already done, so assume $m = 1, 2, \ldots$

$P_n^m(s)$ satisfies $((1-s^2)y')' + \Big(n(n+1) - \dfrac{m^2}{1-s^2}\Big)y = 0$, $y(-1) = y(1) = 0$

Orthogonality follows as usual for e-functions of a self-adjoint e-value problem.

To show completeness, let $q_k(s) = (1-s^2)^{-m/2}P_{m+k}^m(s)$ for $k = 0, 1, 2, \ldots$, so $q_k(s)$ is a polynomial of degree k and $\{q_k(s)\}_{k=0}^{\infty}$ is an orthogonal basis for $L_w^2(-1,1)$ with weight $(1-s^2)^m$; this follows as in the case for $m=0$.

Now suppose $f(s) \in L^2(-1,1)$ is orthogonal to $\{P_{m+k}^m(s)\}_{k=0}^{\infty}$ in $L^2(-1,1)$; then $g(s) = (1-s^2)^{-m/2}f(s) \in L_w^2(-1,1)$ is orthogonal to $\{q_k(s)\}_{k=0}^{\infty}$ in $L_w^2(-1,1)$; so $g(s) = 0$ in $L_w^2(-1,1)$, and hence $f(s) = 0$ in $L^2(-1,1)$. <u>ok</u>

<u>claim</u> : $||P_n^m||^2 = \dfrac{(n+m)!}{(n-m)!}\dfrac{2}{2n+1}$, $n = 0, 1, 2, \ldots$, $m = 0 : n$ ($m = 0$ <u>ok</u>)

<u>pf</u> : set $y_m(s) = P_n^m(s) = (1-s^2)^{m/2}\dfrac{d^m}{ds^m}P_n(s)$, $y_0(s) = P_n(s)$

we will derive a relation between y_m and y_{m-1}

<u>case 1</u> : $m = 1 \Rightarrow y_1 = (1-s^2)^{1/2}y_0'$

$$||y_1||^2 = \int_{-1}^{1}(1-s^2)(y_0')^2ds = \cancelto{0}{(1-s^2)y_0'y_0}\Big|_{-1}^{1} - \int_{-1}^{1}\big((1-s^2)y_0'\big)'y_0ds$$

$$= \int_{-1}^{1} n(n+1)y_0^2ds = n(n+1)||y_0||^2 \quad \underline{\text{ok}}$$

<u>case 2</u> : $m = 2, 3, \ldots \Rightarrow y_{m-1}' = \dfrac{d}{ds}\Big((1-s^2)^{(m-1)/2}\dfrac{d^{m-1}}{ds^{m-1}}P_n\Big)$

$$= (1-s^2)^{(m-1)/2}\frac{d^m}{ds^m}P_n + \frac{m-1}{2}(1-s^2)^{(m-3)/2}(-2s)\frac{d^{m-1}}{ds^{m-1}}P_n$$

$$= (1-s^2)^{-1/2} y_m - (m-1)s(1-s^2)^{-1} y_{m-1}$$

$$y_m = \frac{(m-1)s}{(1-s^2)^{1/2}}\, y_{m-1} + (1-s^2)^{1/2} y'_{m-1}$$

$$||y_m||^2 = \int_{-1}^{1} \left(\frac{(m-1)^2 s^2}{1-s^2} y_{m-1}^2 + (1-s^2)(y'_{m-1})^2 + 2(m-1) s y_{m-1} y'_{m-1} \right) ds$$

integrate 2nd and 3rd terms by parts

$$\int_{-1}^{1} (1-s^2)(y'_{m-1})^2 ds = \cancelto{0}{(1-s^2) y'_{m-1} y_{m-1}}\Big|_{-1}^{1} - \int_{-1}^{1} \big((1-s^2) y'_{m-1}\big)' y_{m-1} ds$$

$$= \int_{-1}^{1} \left(n(n+1) - \frac{(m-1)^2}{1-s^2} \right) y_{m-1}^2 ds$$

$$\int_{-1}^{1} s y_{m-1} y'_{m-1} ds = \cancelto{0}{s y_{m-1}^2\Big|_{-1}^{1}} - \int_{-1}^{1} (s y_{m-1})' y_{m-1} ds$$

$$= -\int_{-1}^{1} \big(s y'_{m-1} y_{m-1} + y_{m-1}^2 \big) ds \Rightarrow 2 \int_{-1}^{1} s y_{m-1} y'_{m-1} ds = -\int_{-1}^{1} y_{m-1}^2 ds$$

$$||y_m||^2 = \int_{-1}^{1} \left(\frac{(m-1)^2 s^2}{1-s^2} + n(n+1) - \frac{(m-1)^2}{1-s^2} - (m-1) \right) y_{m-1}^2 ds$$

$$= (n(n+1) - (m-1)^2 - (m-1)) ||y_{m-1}||^2 = (n(n+1) - (m-1)m) ||y_{m-1}||^2$$

$||y_m||^2 = (n+m)(n-m+1)||y_{m-1}||^2$, agrees with $m = 1$ result

replace m by $m-1, \ldots, 1$

$$||y_m||^2 = (n+m)(n+m-1)\cdots(n+1)\cdot(n-m+1)(n-m+2)\cdots n ||y_0||^2$$

$$= (n+m)(n+m-1)\cdots(n+1)\cdot n(n-1)\cdots(n-m+1)||y_0||^2$$

$$= \frac{(n+m)!}{(n-m)!} ||y_0||^2 \quad \underline{\text{ok}}$$

<u>note</u>

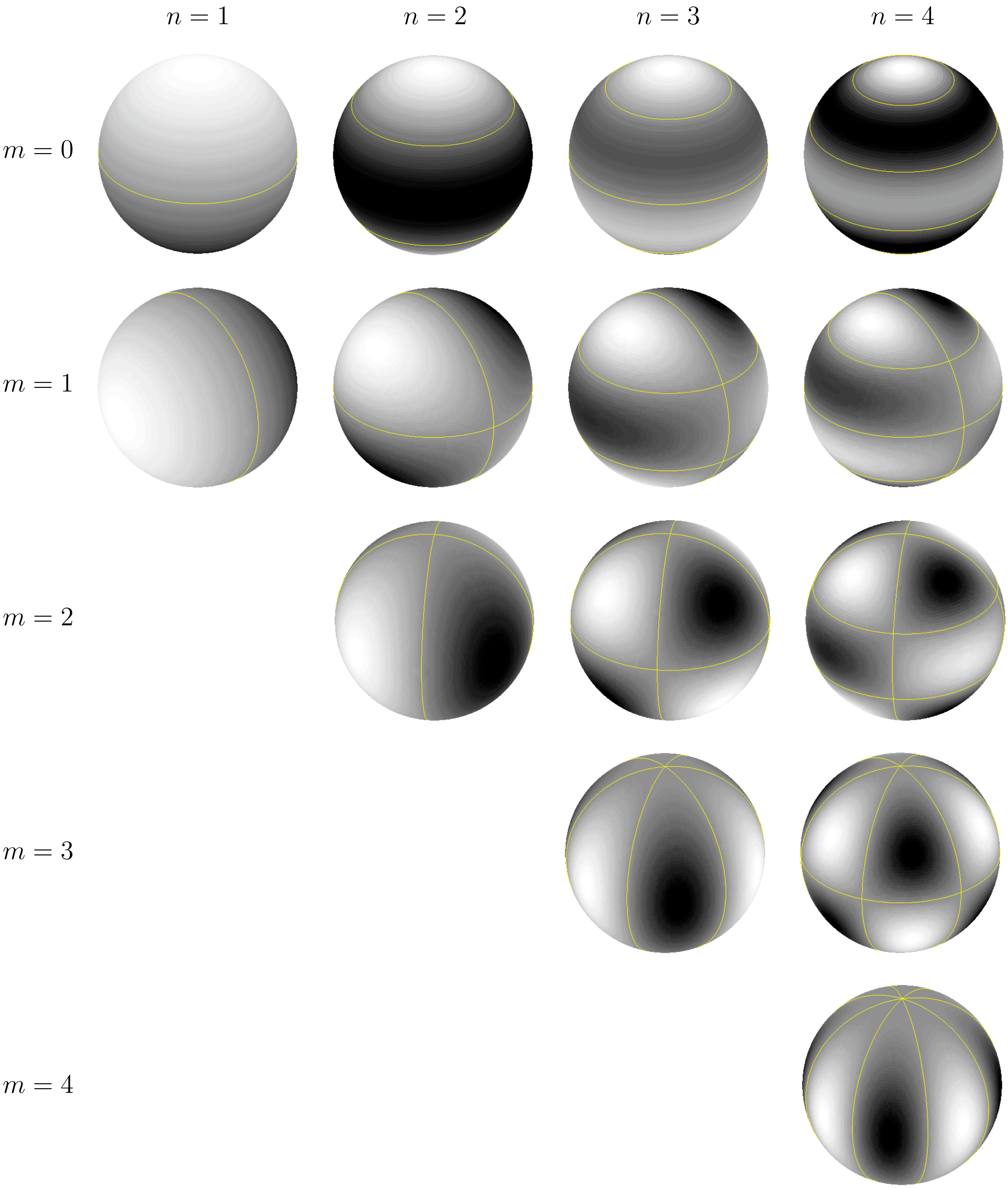
1. $s = \cos\theta \Rightarrow \displaystyle\int_{-1}^{1} f(s)\overline{g(s)} ds = \int_{0}^{\pi} f(\cos\theta)\overline{g(\cos\theta)} \sin\theta d\theta$

2. The unit sphere is a product space, $S = [0,\pi] \times [-\pi,\pi]$.

define $Y_n^m(\theta,\phi) = \sqrt{\dfrac{2n+1}{4\pi} \dfrac{(n-|m|)!}{(n+|m|)!}}\, P_n^{|m|}(\cos\theta) e^{im\phi}$: <u>spherical harmonics</u>

Then $\{Y_n^m(\theta,\phi) : n = 0,1,2,\ldots, m = -n : n\}$ is an orthonormal basis for $L_2(S)$ wrt the surface measure $dS(x) = \sin\theta d\theta d\phi$ for $x = (1,\theta,\phi) \in S$.

spherical harmonics



general solution of $\nabla^2\Phi = 0$ (allowing a singularity at $r = 0$)

$$\Phi(r,\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\Big(a_{mn}r^n + \frac{b_{mn}}{r^{n+1}}\Big)Y_n^m(\theta,\phi)$$

example: interior Dirichlet problem for the unit ball in $\mathbb{R}^3$

Find $\Phi(r,\theta,\phi)$ such that $\nabla^2\Phi = 0$ for $r < 1$ and $\Phi = f$ for $r = 1$.

$$f(\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} a_{mn}Y_n^m(\theta,\phi)\ ,\ a_{mn} = \langle f, Y_n^m\rangle = \int_{-\pi}^{\pi}\int_0^{\pi} f(\theta,\phi)Y_n^{-m}(\theta,\phi)\sin\theta d\theta d\phi$$

$$\Phi(r,\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} a_{mn}r^nY_n^m(\theta,\phi) \qquad \underline{\text{ok}}$$

alternative : $\Phi(x) = \dfrac{1}{4\pi}\displaystyle\int_S \frac{1-|x|^2}{|x-y|^3}f(y)dS(y)$, where $x, y \in \mathbb{R}^3$, $|x| < 1$, $|y| = 1$

pf : Choose the coordinate system so that $x = (r, 0, *)$ is on the positive z-axis; the ϕ-coordinate is not well-defined, but this does not affect the result.

$$\Phi(r,0,*) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} a_{mn}r^nY_n^m(0,*)\ ,\ \text{recall}:\ P_n^0(1) = 1\,, P_n^{|m|}(1) = 0 \text{ for } m \neq 0$$

$$= \sum_{n=0}^{\infty}\sum_{m=-n}^{n} a_{mn}r^n\sqrt{\frac{2n+1}{4\pi}\frac{(n-|m|)!}{(n+|m|)!}}P_n^{|m|}(1)e^{im*} = \sum_{n=0}^{\infty} a_{0n}r^n\sqrt{\frac{2n+1}{4\pi}}$$

$$a_{0n} = \langle f, Y_n^0\rangle = \int_{-\pi}^{\pi}\int_0^{\pi} f(\theta,\phi)\sqrt{\frac{2n+1}{4\pi}}P_n(\cos\theta)\sin\theta d\theta d\phi$$

$$\Phi(x) = \frac{1}{4\pi}\int_S \sum_{n=0}^{\infty}(2n+1)P_n(\cos\theta)r^nf(y)dS(y)\ ,\ y = (1,\theta,\phi) \in S$$

$$\sum_{n=0}^{\infty}(2n+1)P_n(\cos\theta)r^n = \Big(2r\frac{d}{dr}+1\Big)\sum_{n=0}^{\infty}P_n(\cos\theta)r^n$$

$$= \Big(2r\frac{d}{dr}+1\Big)\frac{1}{(1-2r\cos\theta+r^2)^{1/2}}\ ,\ \text{note}:\ 1-2r\cos\theta+r^2 = |x-y|^2$$

$$= 2r\cdot\frac{-\frac{1}{2}(-2\cos\theta+2r)}{(1-2r\cos\theta+r^2)^{3/2}} + \frac{1}{(1-2r\cos\theta+r^2)^{1/2}}$$

$$= \frac{2r\cos\theta-2r^2+1-2r\cos\theta+r^2}{(1-2r\cos\theta+r^2)^{3/2}} = \frac{1-r^2}{(1-2r\cos\theta+r^2)^{3/2}} = \frac{1-|x|^2}{|x-y|^3} \qquad \underline{\text{ok}}$$

<u>thm</u> : The <u>solid harmonic</u> $r^nY_n^m(\theta,\phi)$ is a homogeneous harmonic polynomial of degree n in the Cartesian coordinates (x,y,z).

recall : $x = r\sin\theta\cos\phi\,,\ y = r\sin\theta\sin\phi\,,\ z = r\cos\theta$

$$Y_n^m(\theta,\phi) \sim P_n^{|m|}(\cos\theta)e^{im\phi}\ ,\ \ P_n^m(s) = (1-s^2)^{m/2}\frac{d^m}{ds^m}P_n(s)$$

<u>$n=0$</u> : $Y_0^0 \sim 1$

<u>$n=1$</u>

$$rY_1^0 \sim rP_1^0(\cos\theta) = r\cos\theta = z$$

$$rY_1^1 \sim rP_1^1(\cos\theta)e^{i\phi} = r\sin\theta(\cos\phi + i\sin\phi) = x+iy$$

$$rY_1^{-1} \sim rP_1^1(\cos\theta)e^{-i\phi} = r\sin\theta(\cos\phi - i\sin\phi) = x-iy$$

<u>$n=2$</u>

$$r^2Y_2^0 \sim r^2P_2^0(\cos\theta) \sim r^2(3\cos^2\theta - 1) = 3z^2 - r^2 = 2z^2 - x^2 - y^2$$

$$r^2Y_2^1 \sim r^2P_2^1(\cos\theta)e^{i\phi} \sim r^2\sin\theta\cos\theta(\cos\phi + i\sin\phi) = xz + iyz$$

$$r^2Y_2^2 \sim r^2P_2^2(\cos\theta)e^{2i\phi} \sim r^2\sin^2\theta(\cos\phi + i\sin\phi)^2 = x^2 - y^2 + 2ixy$$

<u>pf</u> : assume $m \ge 0$

recall : $(n+1)P_{n+1}(x) - (2n+1)xP_n(x) + nP_{n-1}(x) = 0\,, P_0(x) = 1\,, P_1(x) = x$

Hence if n is even/odd, then $P_n(x)$ is even/odd.

$$\frac{d^m}{ds^m}P_n(s) = \sum_j a_j s^{n-m-2j}\ \ \text{, where } j \text{ is such that } 0 \le 2j \le n-m$$

$$P_n^m(\cos\theta) = \sin^m\theta\cdot\sum_j a_j(\cos\theta)^{n-m-2j}$$

$$r^nP_n^m(\cos\theta)e^{im\phi} = r^n\sin^m\theta\cdot\sum_j a_j(\cos\theta)^{n-m-2j}e^{im\phi}$$

$$= (r\sin\theta e^{i\phi})^m\cdot\sum_j a_j r^{2j}(r\cos\theta)^{n-m-2j}$$

$$= (x+iy)^m\cdot\sum_j a_j(x^2+y^2+z^2)^j z^{n-m-2j}\ \ \text{, similarly for } m<0 \quad \underline{\text{ok}}$$

1. Hence $Y_n^m(\theta,\phi)$ is the restriction of a homogeneous harmonic polynomial in (x,y,z) to the unit sphere.

2. $$\Phi(r,\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} a_{mn}r^nY_n^m(\theta,\phi) = \sum_{n=0}^{\infty} a_{n_1n_2n_3}x^{n_1}y^{n_2}z^{n_3}\begin{cases} n = n_1+n_2+n_3 \\ 0 \le n_i \le n \\ \text{Taylor series in } x,y,z \end{cases}$$

recall : $\dfrac{P_n(\cos\theta)}{r^{n+1}} = \dfrac{(-1)^n}{n!}\partial_z^n(r^{-1})$: multipole potential of order 2^n along z-axis

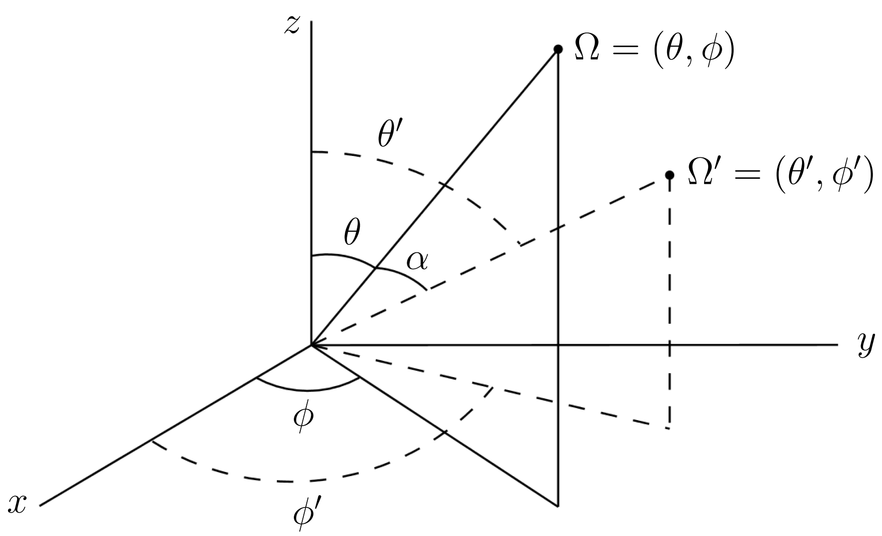
in general : $\dfrac{P_n^{|m|}(\cos\theta)}{r^{n+1}}\, e^{\pm im\phi} = \dfrac{(-1)^n}{(n-m)!}\,\partial_\pm^m \partial_z^{n-m}(r^{-1})$, $\partial_\pm = \partial_x \pm i\partial_y$, pf ...

<u>addition formula</u> for spherical harmonics (Wallace ...)

$$f(\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} c_{mn}\, Y_n^m(\theta,\phi)\ ,\ c_{mn} = \int_S f(\theta',\phi')\,\overline{Y_n^m}(\theta',\phi')d\Omega'\ ,\ d\Omega' = \sin\theta' d\theta' d\phi'$$

$$f(\theta,\phi) = \int_S f(\theta',\phi')\sum_{n=0}^{\infty}\sum_{m=-n}^{n} Y_n^m(\theta,\phi)\,\overline{Y_n^m}(\theta',\phi')d\Omega'$$

$$\Rightarrow \sum_{n=0}^{\infty}\sum_{m=-n}^{n} Y_n^m(\theta,\phi)\,\overline{Y_n^m}(\theta',\phi') = \delta(\Omega-\Omega')$$



Consider the line through Ω as a new z-axis; then $\Omega \to (0,*), \Omega' \to (\alpha,\beta)$.
Then α is the angle from Ω to Ω'; so if $\phi = \phi'$, then $\alpha = \theta' - \theta$, but in general $\alpha = \alpha(\theta,\phi,\theta',\phi')$.

<u>claim</u>

1. $\cos\alpha \ = \ \cos\theta\cos\theta' \ + \ \sin\theta\sin\theta'\cos(\phi-\phi')$

2. $P_n(\cos\alpha) = \dfrac{4\pi}{2n+1}\displaystyle\sum_{m=-n}^{n} Y_n^m(\theta,\phi)\,\overline{Y_n^m}(\theta',\phi')$: addition formula

<u>pf</u> : 1. $\Omega = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, $\Omega' = (\sin\theta'\cos\phi', \sin\theta'\sin\phi', \cos\theta')$

$\cos\alpha = \Omega\cdot\Omega' = \sin\theta\cos\phi\sin\theta'\cos\phi' + \sin\theta\sin\phi\sin\theta'\sin\phi' + \cos\theta\cos\theta'$

$\quad = \sin\theta\sin\theta'(\cos\theta\cos\theta' + \sin\phi\sin\phi') + \cos\theta\cos\theta'$ <u>ok</u>

2. $\displaystyle\sum_{n=0}^{\infty}\sum_{m=-n}^{n} Y_n^m(\theta,\phi)\,\overline{Y_n^m}(\theta',\phi') = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} Y_n^m(0,*)\,\overline{Y_n^m}(\alpha,\beta)$

$$\Rightarrow Y_n^m(0,*) = \sqrt{\frac{2n+1}{4\pi}\frac{(n-|m|)!}{(n+|m|)!}}\,P_n^{|m|}(1)e^{im*}\,,\ P_n^{|m|}(1) = \begin{cases}1, & m=0\\ 0, & m\neq 0\end{cases}$$

$$Y_n^0(0,*) = \sqrt{\frac{2n+1}{4\pi}}\ ,\ Y_n^0(\alpha,\beta)\ =\ \sqrt{\frac{2n+1}{4\pi}}P_n(\cos\alpha)$$

$$\sum_{n=0}^{\infty}\sum_{m=-n}^{n} Y_n^m(\theta,\phi)\,\overline{Y_n^m}(\theta',\phi') = \sum_{n=0}^{\infty}\frac{2n+1}{4\pi}P_n(\cos\alpha)\ \ldots\quad \underline{\text{ok}}$$

<u>application</u> : $\nabla^2\Phi = 4\pi\rho \Rightarrow \Phi(x) = \displaystyle\int_{\mathbb{R}^3}\frac{\rho(x')}{|x-x'|}\,dx'\,,\ \begin{cases}x=(r,\theta,\phi)\\ x'=(r',\theta',\phi')\end{cases}$

$$\frac{1}{|x-x'|}\ =\ \frac{1}{\sqrt{r^2-2rr'\cos\alpha+(r')^2}} = \sum_{n=0}^{\infty}\frac{r_<^n}{r_>^{n+1}}P_n(\cos\alpha)\,,\ \begin{cases}r_< = \min(r,r')\\ r_> = \max(r,r')\end{cases}$$

<u>case 1</u> : $\rho(x) = 0$ for $|x| > R$

$$\Phi(x) = \int_S\int_0^R \rho(x')\sum_{n=0}^{\infty}\frac{(r')^n}{r^{n+1}}P_n(\cos\alpha)(r')^2dr'd\Omega'\ \ ,\ \text{for } r > R$$

$$= \int_S\int_0^R \rho(x')\sum_{n=0}^{\infty}\frac{(r')^n}{r^{n+1}}\frac{4\pi}{2n+1}\sum_{m=-n}^{n} Y_n^m(\theta,\phi)\,\overline{Y_n^m}(\theta',\phi')(r')^2dr'd\Omega'$$

$$\Phi(x) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{a_{mn}}{r^{n+1}}Y_n^m(\theta,\phi)\ :\ \text{multipole expansion , valid for } |x| > R$$

$$a_{mn} = \frac{4\pi}{2n+1}\int_S\int_0^R \rho(x)r^n\overline{Y_n^m}(\theta,\phi)dx\ :\ \text{multipole moments}$$

<u>case 2</u> : $\rho(x) = 0$ for $|x| < R$

$$\Phi(x) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} b_{mn}r^nY_n^m(\theta,\phi)\ :\ \text{local expansion , valid for } |x| < R$$

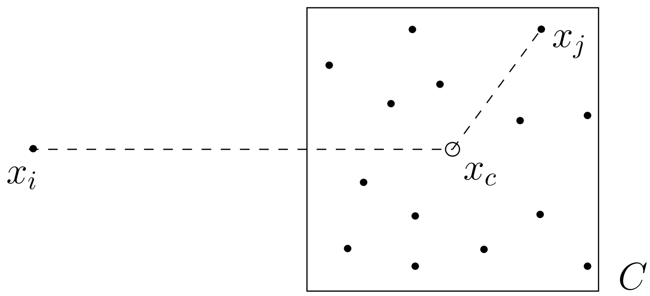
$$b_{mn} = \frac{4\pi}{2n+1}\int_S\int_R^{\infty}\rho(x)\frac{1}{r^{n+1}}\overline{Y_n^m}(\theta,\phi)dx\ :\ \text{local coefficients}$$

<u>application of multipole expansion</u> : improve accuracy of BH treecode

$$V = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \frac{q_i q_j}{|x_i - x_j|} \ : \ \text{direct sum} = O(N^2)$$

$$V = \frac{1}{2} \sum_{i=1}^{N} q_i \Phi_i \ , \ \Phi_i = \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{q_j}{|x_i - x_j|} = \sum_{C} \sum_{x_j \in C} \frac{q_j}{|x_i - x_j|} = \sum_{C} \Phi_{i,C}$$

$$\Phi_{i,C} = \sum_{x_j \in C} \frac{q_j}{|x_i - x_j|} \ : \ \text{particle-cluster interaction} \begin{cases} \text{three options} \\ \text{1. direct sum} \\ \text{2. multipole approximation} \\ \text{3. consider children} \end{cases}$$



x_i : target particle

x_j : source particle

2a. $\Phi_{i,C} \approx \dfrac{Q_C}{|x_i - x_c|} \ , \ Q_C = \displaystyle\sum_{x_j \in C} q_j$: monopole approximation

2b. $\Phi_{i,C} \approx \displaystyle\sum_{n=0}^{p} \sum_{m=-n}^{n} \frac{M_n^m}{r_i^{n+1}} Y_n^m(\theta_i, \phi_i)$: multipole approximation

$$x_i - x_c = (r_i, \theta_i, \phi_i) \ , \ x_j - x_c = (r_j, \theta_j, \phi_j)$$

$$\begin{aligned} M_n^m &= \frac{4\pi}{2n+1} \int_{\mathbb{R}^3} \rho(x) r^n \overline{Y_n^m}(\theta, \phi) dx \\ &= \frac{4\pi}{2n+1} \int_{\mathbb{R}^3} \sum_{x_j \in C} q_j \delta(x - x_j) r^n \overline{Y_n^m}(\theta, \phi) dx \\ &= \frac{4\pi}{2n+1} \sum_{x_j \in C} q_j r_j^n \, \overline{Y_n^m}(\theta_j, \phi_j) \ : \ \text{multipole moments of cluster } C \end{aligned}$$

1. $p = 0 \Rightarrow$ monopole approximation

2. A pth order particle-cluster approximation requires $O(p^2)$ moments; the cost of computing each moment is $O(N_c)$, but they can be stored and reused for different target particles x_i; then the operation count for a pth order multipole approximation is $O(p^2)$, and this yields a pth order treecode with operation count $O(N \log N)$.

error bound for multipole approximation

$$\left|\Phi_{i,C} - \sum_{n=0}^{p}\sum_{m=-n}^{n} \frac{M_n^m}{r_i^{n+1}} Y_n^m(\theta_i,\phi_i)\right| \le \frac{A}{r_i - a}\left(\frac{a}{r_i}\right)^{p+1}, \text{ where } \Phi_{i,C} = \sum_{x_j \in C} \frac{q_j}{|x_i - x_j|}$$

$A = \sum_{x_j \in C} |q_j|$: absolute cluster charge , $a = \max_j |r_j|$: cluster radius

pf : $$\sum_{m=-n}^{n} \frac{M_n^m}{r_i^{n+1}} Y_n^m(\theta_i,\phi_i) = \sum_{m=-n}^{n} \frac{4\pi}{2n+1} \sum_{x_j\in C} q_j r_j^n \overline{Y_n^m}(\theta_j,\phi_j) \frac{1}{r_i^{n+1}} Y_n^m(\theta_i,\phi_i)$$

$$= \sum_{x_j\in C} q_j \frac{r_j^n}{r_i^{n+1}} \frac{4\pi}{2n+1} \sum_{m=-n}^{n} Y_n^m(\theta_i,\phi_i)\overline{Y_n^m}(\theta_j,\phi_j) = \sum_{x_j\in C} q_j \frac{r_j^n}{r_i^{n+1}} P_n(\cos\alpha_{ij})$$

recall : $$\frac{1}{|x_i - x_j|} = \sum_{n=0}^{\infty} \frac{r_j^n}{r_i^{n+1}} P_n(\cos\alpha_{ij}) \text{ for } r_j < r_i$$

$$\left|\frac{1}{|x_i - x_j|} - \sum_{n=0}^{p} \frac{r_j^n}{r_i^{n+1}} P_n(\cos\alpha_{ij})\right| \le \sum_{n=p+1}^{\infty} \frac{r_j^n}{r_i^{n+1}} |P_n(\cos\alpha_{ij})| \le \sum_{n=p+1}^{\infty} \frac{r_j^n}{r_i^{n+1}}$$

$$\le \frac{1}{r_i}\left(\frac{r_j}{r_i}\right)^{p+1} \frac{1}{1 - r_j/r_i} = \left(\frac{r_j}{r_i}\right)^{p+1} \frac{1}{r_i - r_j} \le \left(\frac{a}{r_i}\right)^{p+1} \frac{1}{r_i - a} \quad \underline{\text{ok}}$$

---

claim : $$P_n(s) = \frac{1}{2\pi}\int_0^{2\pi} \left(s + i\sqrt{1-s^2}\sin\theta\right)^n d\theta \text{ (then } |P_n(s)| \le 1 \text{ for } |s| \le 1)$$

pf : $$P_n(s) = \frac{1}{2^n n!}\frac{d^n}{ds^n}(s^2-1)^n = \frac{1}{2^n n!}\frac{n!}{2\pi i}\int_C \frac{(z^2-1)^n}{(z-s)^{n+1}}\,dz$$

assume $-1 < s < 1$, let $C : z = s + \sqrt{1-s^2}\, e^{i\theta}$, $0 \le \theta \le 2\pi$

$z - s = \sqrt{1-s^2}\, e^{i\theta}$, $dz = \sqrt{1-s^2}\, ie^{i\theta} d\theta$

$$z^2 - 1 = s^2 + (1-s^2)e^{2i\theta} + 2s\sqrt{1-s^2}\, e^{i\theta} - 1$$

$$= \sqrt{1-s^2}\, e^{i\theta}\left(2s + \sqrt{1-s^2}\, e^{i\theta} - \sqrt{1-s^2}\, e^{-i\theta}\right)$$

$$= \sqrt{1-s^2}\, e^{i\theta} 2\left(s + i\sqrt{1-s^2}\sin\theta\right)$$

$$P_n(s) = \frac{1}{2^n}\frac{1}{2\pi i}\int_0^{2\pi} \frac{(1-s^2)^{n/2} e^{in\theta} 2^n \left(s + i\sqrt{1-s^2}\sin\theta\right)^n}{(1-s^2)^{(n+1)/2} e^{i(n+1)\theta}} \sqrt{1-s^2}\, ie^{i\theta} d\theta \quad \underline{\text{ok}}$$

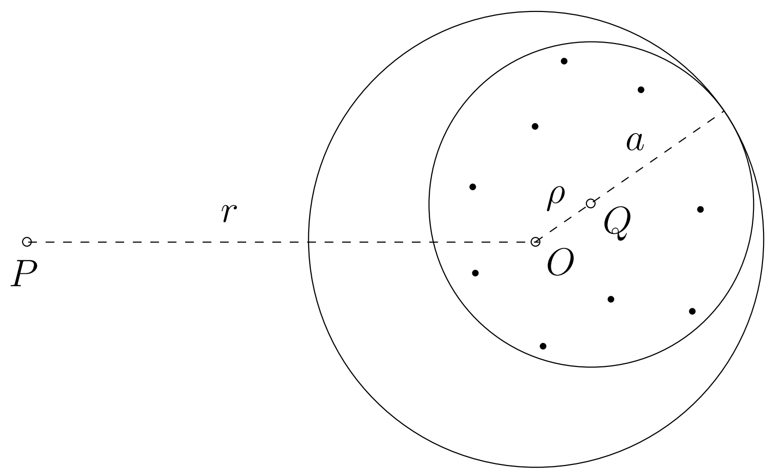
<u>fast multipole method</u> : Greengard-Rokhlin (1987, ...)

idea : evaluate local approximation due to combined multipole approximations

note : $Y_n^m(\theta,\phi) = \sqrt{\dfrac{(n-|m|)!}{(n+|m|)!}} P_n^{|m|}(\cos\theta)e^{im\phi}$, $A_n^m = \dfrac{(-1)^n}{\sqrt{(n-|m|)!(n+|m|)!}}$

<u>three tools</u>

Consider point charges $x_1,\ldots,x_N$ inside a sphere of radius a centered at Q and also inside a sphere of radius $\rho + a$ centered at O, and let P be a point outside the 2nd sphere.



coordinates at O
$P - O = (r,\theta,\phi)$
$x_i - O = (r_i,\theta_i,\phi_i)$
$Q - O = (\rho,\alpha,\beta)$
assume $r > \rho + a$
coordinates at Q
$P - Q = (r',\theta',\phi')$
$x_i - Q = (r_i',\theta_i',\phi_i')$

1. shift the center of a multipole expansion (M2M)

$$\Phi(P) = \sum_{i=1}^{N} \frac{q_i}{|P-x_i|} \ : \ \text{induced potential at } P$$

$$= \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \frac{Q_n^m}{(r')^{n+1}} Y_n^m(\theta',\phi') \ : \ \text{multipole expansion at } Q$$

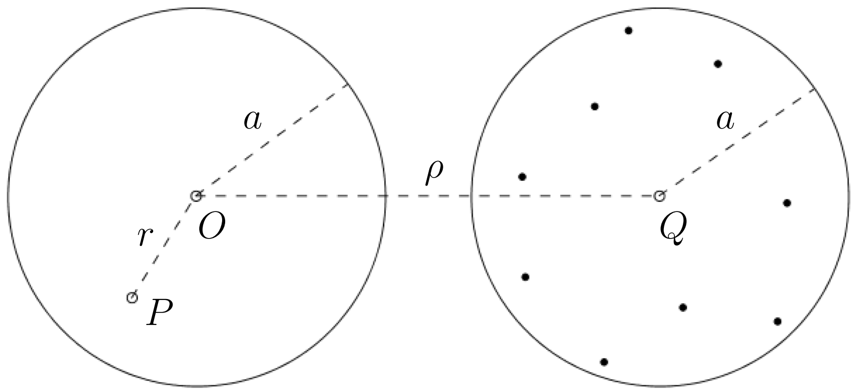
$$Q_n^m = \sum_{i=1}^{N} q_i\,(r_i')^n\,\overline{Y_n^m}(\theta_i',\phi_i') \ : \ \text{multipole moments at } Q$$

$$\Phi(P) = \sum_{l=0}^{\infty}\sum_{k=-l}^{l} \frac{O_l^k}{r^{l+1}} Y_l^k(\theta,\phi) \ : \ \text{multipole expansion at } O$$

$$O_l^k = \sum_{i=1}^{N} q_i\,r_i^l\,\overline{Y_l^k}(\theta_i,\phi_i) \ : \ \text{multipole moments at } O$$

$$O_l^k = \sum_{n=0}^{l}\sum_{m=-n}^{n} Q_{l-n}^{k-m}\, \frac{i^{|k|-|m|-|k-m|}\,A_n^m\,A_{l-n}^{k-m}}{A_l^k}\,\rho^n\,\overline{Y_n^m}(\alpha,\beta)$$

2. convert a multipole expansion to a local expansion (M2L)



coordinates at O
$P - O = (r, \theta, \phi)$
$x_i - O = (r_i, \theta_i, \phi_i)$
$Q - O = (\rho, \alpha, \beta)$
assume $\rho > 2a$, $r < a$
coordinates at Q
$P - Q = (r', \theta', \phi')$
$x_i - Q = (r'_i, \theta'_i, \phi'_i)$

$$\Phi(P) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{Q_n^m}{(r')^{n+1}} Y_n^m(\theta', \phi') \ : \ \text{multipole expansion at } Q$$

$$= \sum_{l=0}^{\infty} \sum_{k=-l}^{l} O_l^k r^l Y_l^k(\theta, \phi) \ : \ \text{local expansion at } O$$

$$O_l^k = \sum_{i=1}^{N} q_i \frac{1}{r_i^{l+1}} \overline{Y_l^k}(\theta_i, \phi_i) \ : \ \text{local coefficients at } O$$

$$O_l^k = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} Q_n^m \frac{i^{|k-m|-|k|-|m|} A_n^m A_l^k}{(-1)^n A_{l+n}^{m-k}} \frac{1}{\rho^{l+n+1}} Y_{l+n}^{m-k}(\alpha, \beta)$$

If the sum is truncated at order p, the operation count for each M2L is $O(p^4)$.

---

3. shift the center of a local approximation (L2L)

No assumptions for r, ρ, a are needed in this case.

$$\Phi(P) = \sum_{n=0}^{p} \sum_{m=-n}^{n} Q_n^m (r')^n Y_n^m(\theta', \phi') \ : \ \text{local approximation at } Q$$

$$= \sum_{l=0}^{p} \sum_{k=-l}^{l} O_l^k r^l Y_l^k(\theta, \phi) \ : \ \text{local approximation at } O$$

$$O_l^k = \sum_{n=l}^{p} \sum_{m=-n}^{n} Q_n^m \frac{i^{|m|-|m-k|-|k|} A_{n-l}^{m-k} A_l^k}{(-1)^{n+l} A_n^m} \rho^{n-l} Y_{n-l}^{m-k}(\alpha, \beta)$$

<u>example</u> : $ax^2 + bx + c \ = \ a'(x - x_0)^2 + b'(x - x_0) + c'$

def : Two boxes at the same level are neighbors if they share a boundary point; otherwise they are well-separated. The interaction list of a box b contains the children of the neighbors of b's parent that are well-separated from b.

n	n	n	i
n	b	n	i
n	n	n	i
i	i	i	i

i	i	i	i	i	i		
i	i	i	i	i	i		
i	i	n	n	n	i		
i	i	n	b	n	i		
i	i	n	n	n	i		
i	i	i	i	i	i		

note : #(interaction list) $= 3^2 \cdot 4 - 3^2 = 27$ in 2D , $3^3 \cdot 8 - 3^3 = 189$ in 3D

FMM algorithm

1. upward pass

a. Form multipole moments of each box on finest level of tree.

b. Form multipole moments of each parent by shifting multipole moments of children to center of parent using M2M and adding them together.

2. downward pass

a. Starting at coarsest level of tree, convert multipole moments of each box b into local coefficients at the center of each box b_i in b's interaction list using M2L; combine local coefficients in b_i from different boxes b.

b. Starting at coarsest level of tree, shift local coefficients of each parent to center of each child using L2L and add to local coefficients of child.

c. At finest level of tree, evaluate local expansion at each particle and add result to direct interactions with neighbor particles.

operation count

The bulk of the work is due to M2L. Assume there are s particles per box at the finest level and hence N/s boxes at that level. Then the cost of M2L is bounded by $189 \cdot p^4 \cdot \dfrac{N}{s} \cdot \left(1 + \dfrac{1}{8} + \dfrac{1}{8^2} \cdots\right) = O(N)$.

<u>note</u>

Various techniques have been developed to extend or improve the FMM.

1. Poisson integral formula (Anderson 1992)

2. plane-wave expansions (GR 1997)

$$\frac{1}{r} = \frac{1}{\sqrt{x^2+y^2+z^2}} = \frac{1}{2\pi}\int_0^\infty \int_0^{2\pi} e^{-\lambda(z-ix\cos\alpha - iy\sin\alpha)}\, d\alpha\, d\lambda \text{ , valid for } z>0$$

$$\sum_{n=0}^{p}\sum_{m=-n}^{n} \frac{M_n^m}{r^{n+1}} Y_n^m(\theta,\phi) \;\to\; \sum_{j=1}^{J}\sum_{k=1}^{K_j} e^{-\lambda_j(z-ix\cos\alpha_k - iy\sin\alpha_k)} w_{jk}$$

3. kernel-independent FMM (Ying, Biros, Zorin, 2004)

There have also been improvements to the BH treecode.

Draghicescu[2] (1995) , Lindsay, Duan, K (2000, ...)

$$\Phi_{i,C} = \sum_{x_j\in C} \frac{q_j}{|x_i - x_j|} \text{ : particle-cluster interaction , set } g(x,y) = \frac{1}{|x-y|}$$

$$= \sum_{x_j\in C} q_j g(x_i,x_j) = \sum_{x_j\in C} q_j g(x_i, x_c + (x_j - x_c))$$

$$= \sum_{x_j\in C} q_j \sum_{||k||=0}^{\infty} \frac{1}{k!} D_y^k g(x_i,x_c)(x_j-x_c)^k \text{ : Cartesian Taylor expansion}$$

<u>multi-index notation</u>

$k = (k_1,k_2,k_3)\,,\ k_i \geq 0\,,\ ||k|| = k_1+k_2+k_3\,,\ k! = k_1!\,k_2!\,k_3!$

$y = (y_1,y_2,y_3)\,,\ D_y^k = D_{y_1}^{k_1} D_{y_2}^{k_2} D_{y_3}^{k_3}$

$(x_j - x_c)^k = (x_{j,1}-x_{c,1})^{k_1}(x_{j,2}-x_{c,2})^{k_2}(x_{j,3}-x_{c,3})^{k_3}$

<u>Cartesian multipole expansion</u>

$$\Phi_{i,C} = \sum_{||k||=0}^{\infty} M_C^k\, a_k(x_i,x_c)\,,\ M_C^k = \sum_{x_j\in C} q_j(x_j-x_c)^k\,,\ a_k(x_i,x_c) = \frac{1}{k!}D_y^k g(x_i,x_c)$$

compare to spherical form , $x_i - x_c = (r_i,\theta_i,\phi_i)$, $x_j - x_c = (r_j,\theta_j,\phi_j)$

$$\Phi_{i,C} = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \frac{M_n^m}{r_i^{n+1}} Y_n^m(\theta_i,\phi_i) \text{ , } M_n^m = \sum_{x_j\in C} q_j r_j^n \overline{Y_n^m}(\theta_j,\phi_j)$$

<u>note</u>

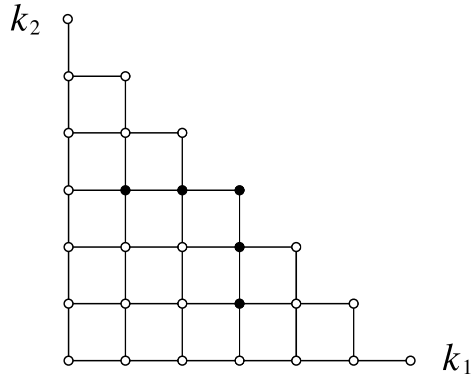
In Cartesian form we obtain a pth order particle-cluster approximation by retaining terms with $||k|| \leq p$. The Cartesian sum runs over 3 indices (k_1, k_2, k_3) and has $O(p^3)$ terms, while the spherical sum runs over 2 indices (m, n) and has $O(p^2)$ terms.

<u>recurrence relation for Cartesian Taylor coefficients</u>

$$a_k = \frac{1}{k!} D_y^k g(x,y) \ , \ \ g(x,y) = \frac{1}{|x-y|}$$

$$||k|| \cdot |x-y|^2 a_k - \big(2||k|| - 1\big) \sum_{i=1}^{3} (x_i - y_i)\, a_{k-e_i} + \big(||k|| - 1\big) \sum_{i=1}^{3} a_{k-2e_i} = 0$$

<u>stencil</u>



This is a 3D analog of the 1D recurrence relation for the Legendre polynomials; recall : $(n+1)P_{n+1}(x) - (2n+1)xP_n(x) + nP_{n-1}(x) = 0$. There are similar recurrence relations for the following kernels.

$$g(x,y) = |x-y|^\nu \ , \ \ (|x-y|^2 + \delta^2)^{\nu/2} \ , \ \ \frac{\mathrm{erf}(\alpha|x-y|)}{|x-y|} \ , \ \ \frac{e^{-\kappa|x-y|}}{|x-y|}$$

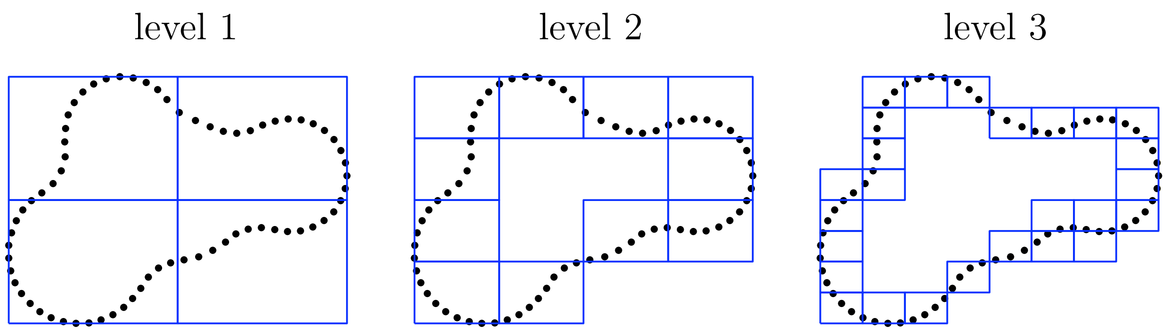
<u>pf</u>

$$g(x,y) = \frac{1}{|x-y|} \ \Rightarrow \ |x-y|^2 g(x,y)^2 = 1 \, , \ \ldots$$

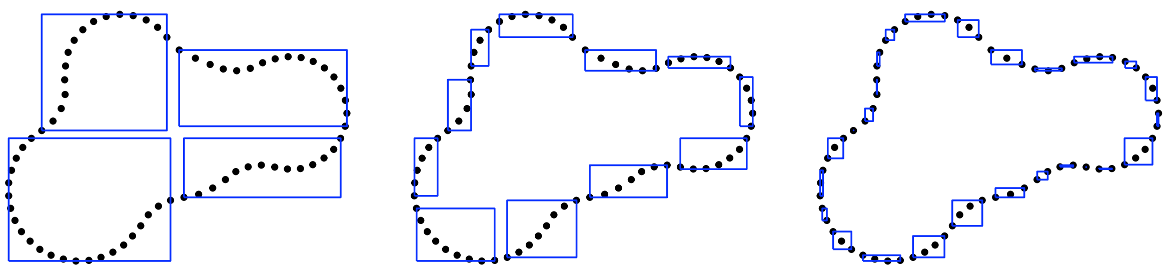
<u>other techniques</u>

1. error criterion : $\dfrac{|M|_p}{R^{p+1}} \leq \epsilon$, $|M|_p = \displaystyle\sum_{x_j \in C} |q_j|\, |x_j - x_c|^p$, $R = |x_i - x_c|$
2. adaptive order
3. compare CPU time for pth order approximation and direct sum
4. adaptive clusters

standard clusters



adaptive clusters

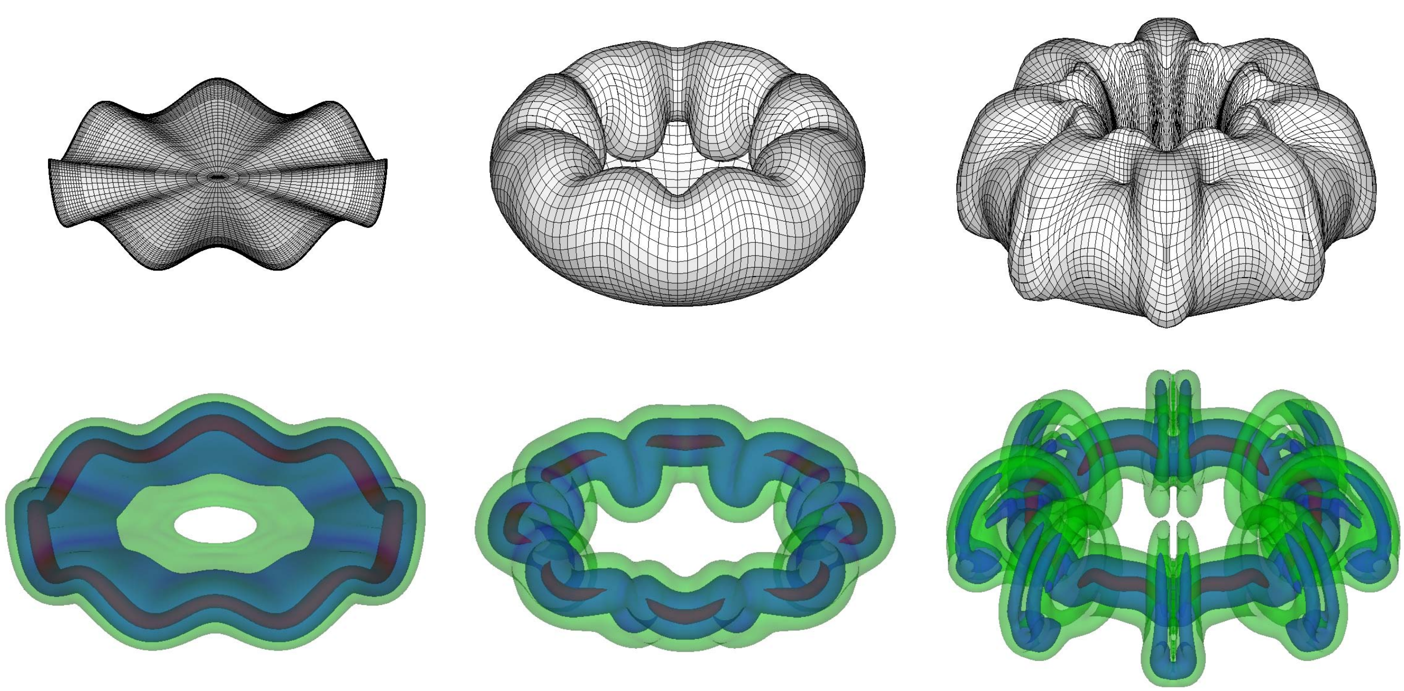


azimuthal waves on a vortex ring (Feng-Kaganovskiy-K 2009)

vortex sheet model , Lagrangian particle/panel method

$N_i \approx 10^4$, $N_f \approx 1.4 \times 10^6$

sheet surface/vorticity isosurfaces at $t = 0, 4, 8$



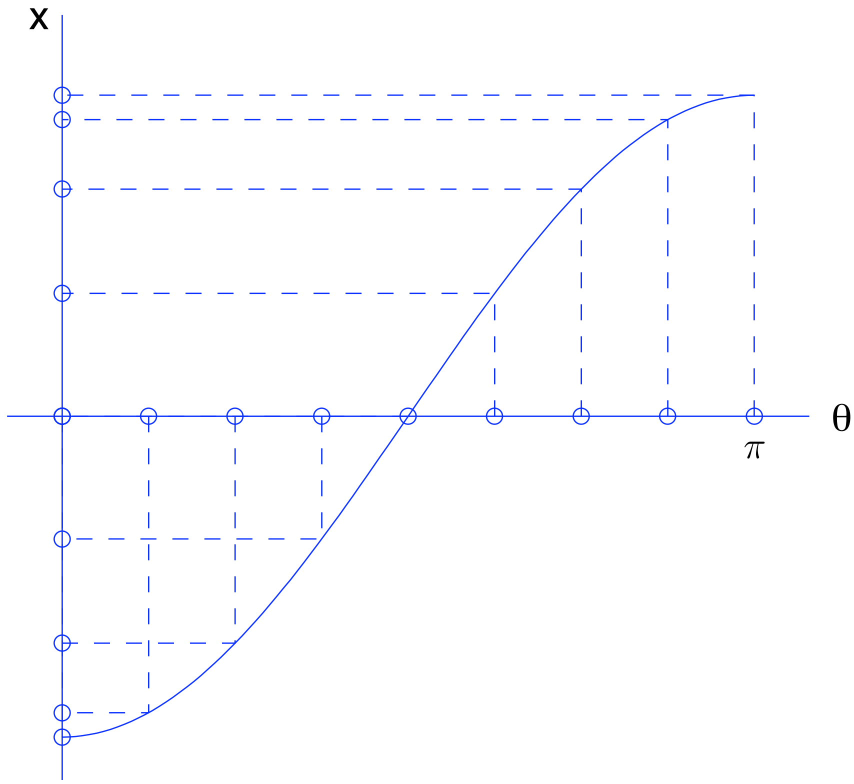
recall : polynomial interpolation in 1D

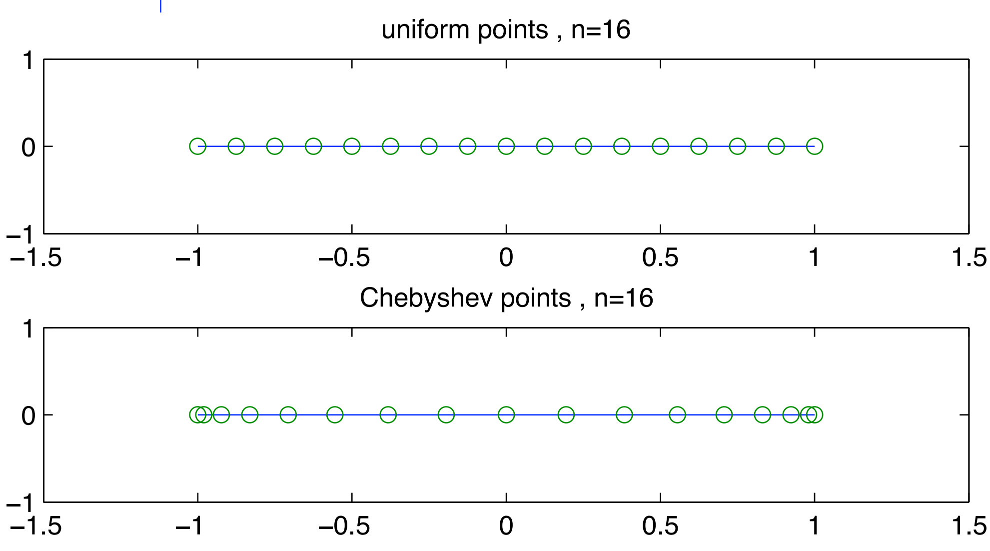
thm : Given $f(x)$ and $n+1$ distinct points $\{s_0, \ldots, s_n\}$ in $[a, b]$, there is a unique polynomial $p(x)$ of degree $\leq n$ that interpolates f at the given points, i.e. such that $p(s_k) = f(s_k)$ for $k = 0 : n$.

question : How should the points be chosen? Consider two options on $[-1, 1]$.

1. uniform points : $s_k = -1 + kh$, $h = 2/n$, $k = 0 : n$

2. Chebyshev points : $s_k = -\cos\theta_k$, $\theta_k = kh$, $h = \pi/n$, $k = 0 : n$



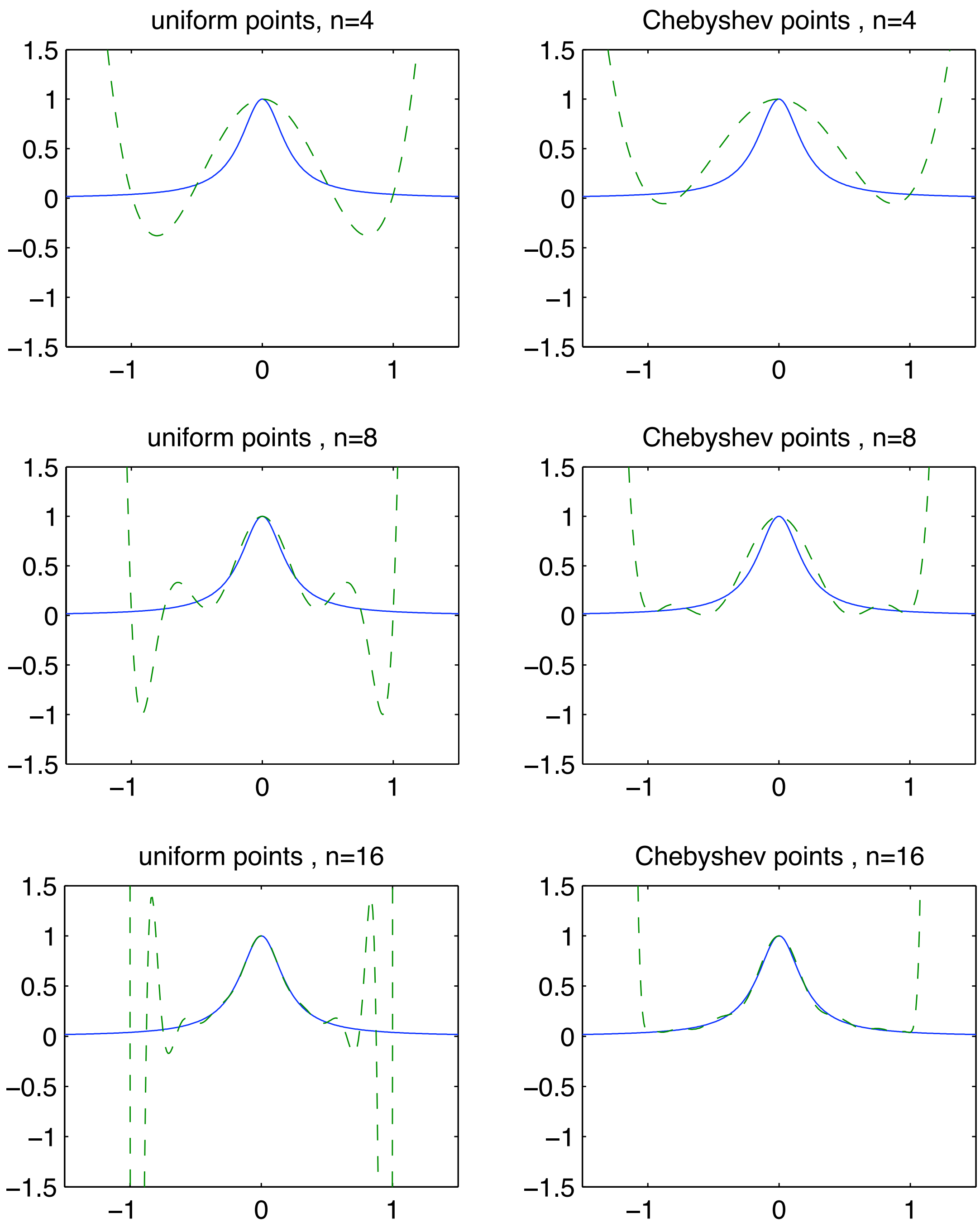


The Chebyshev points are clustered near the endpoints of the interval.

<u>example</u> : $f(x) = \dfrac{1}{1+25x^2}$, $-1 \le x \le 1$

solid line : $f(x)$, given function

dashed line : $p(x)$, interpolating polynomial



1. Interpolation at the uniform points gives a good approximation near the center of the interval, but it gives a bad approximation near the endpoints.

2. Interpolation at the Chebyshev points gives a good approximation on the entire interval.

The interpolating polynomial $p(x)$ can be exressed in different forms.

standard form : $p(x) = a_0 + a_1 x + \cdots + a_n x^n$

Newton form : $p(x) = a_0 + a_1(x - s_0) + a_2(x - s_0)(x - s_1) + \cdots$
$\qquad + a_n(x - s_0)\cdots(x - s_{n-1})$

Lagrange form : $p(x) = \displaystyle\sum_{k=0}^{n} L_k(x) f_k$, $L_k(s_j) = \delta_{jk}$

conventional Lagrange form : $L_k(x) = \dfrac{\Pi_{\substack{j=0\\ j\neq k}}^{n}(x - s_j)}{\Pi_{\substack{j=0\\ j\neq k}}^{n}(s_k - s_j)}$, $k = 0 : n$

barycentric Lagrange form : $L_k(x) = \dfrac{\dfrac{w_k}{x - s_k}}{\displaystyle\sum_{j=0}^{n} \dfrac{w_j}{x - s_j}}$, $w_k = \dfrac{1}{\Pi_{j=0, j\neq k}^{n}(s_k - s_j)}$

<u>example</u> : $n = 2$, $\{s_0, s_1, s_2\}$, $\{f_0, f_1, f_2\}$

$p(x) = L_0(x) f_0 + L_1(x) f_1 + L_2(x) f_2$

$$L_0(x) = \frac{(x - s_1)(x - s_2)}{(s_0 - s_1)(s_0 - s_2)} , \; L_1(x) = \frac{(x - s_0)(x - s_2)}{(s_1 - s_0)(s_1 - s_2)} , \; L_2(x) = \frac{(x - s_0)(x - s_1)}{(s_2 - s_0)(s_2 - s_1)}$$

$$\Rightarrow p(x) = \left(\frac{w_0}{x - s_0} f_0 + \frac{w_1}{x - s_1} f_1 + \frac{w_2}{x - s_2} f_2\right)(x - s_0)(x - s_1)(x - s_2)$$

$$w_0 = \frac{1}{(s_0 - s_1)(s_0 - s_2)} , \; w_1 = \frac{1}{(s_1 - s_0)(s_1 - s_2)} , \; w_2 = \frac{1}{(s_2 - s_0)(s_2 - s_1)}$$

special case : $1 = \left(\dfrac{w_0}{x - s_0} + \dfrac{w_1}{x - s_1} + \dfrac{w_2}{x - s_2}\right)(x - s_0)(x - s_1)(x - s_2)$

$$\Rightarrow p(x) = \frac{\dfrac{w_0}{x - s_0} f_0 + \dfrac{w_1}{x - s_1} f_1 + \dfrac{w_2}{x - s_2} f_2}{\dfrac{w_0}{x - s_0} + \dfrac{w_1}{x - s_1} + \dfrac{w_2}{x - s_2}} \Rightarrow L_k(x) = \frac{\dfrac{w_k}{x - s_k}}{\displaystyle\sum_{j=0}^{2} \dfrac{w_j}{x - s_j}} \qquad \underline{\text{ok}}$$

1. The barycentric Lagrange form of $p(x)$ is <u>scale invariant</u>, i.e. the same weights w_k can be used for any interval $[a, b]$. pf ...

2. If the interpolation points are the Chebyshev points, then the barycentric weights are $w_k = (-1)^k \delta_k$, where $\delta_0 = \delta_n = \frac{1}{2}, \delta_k = 1$ for $k = 1 : n - 1$. pf ...

Berrut-Trefethen (SIREV 2004) : "Barycentric interpolation is a variant of Lagrange polynomial interpolation that is fast and stable. It deserves to be known as the standard method of polynomial interpolation."

<u>extension to 3D</u>

$C = [a_1, b_1] \times [a_2, b_2] \times [a_3, b_3]$

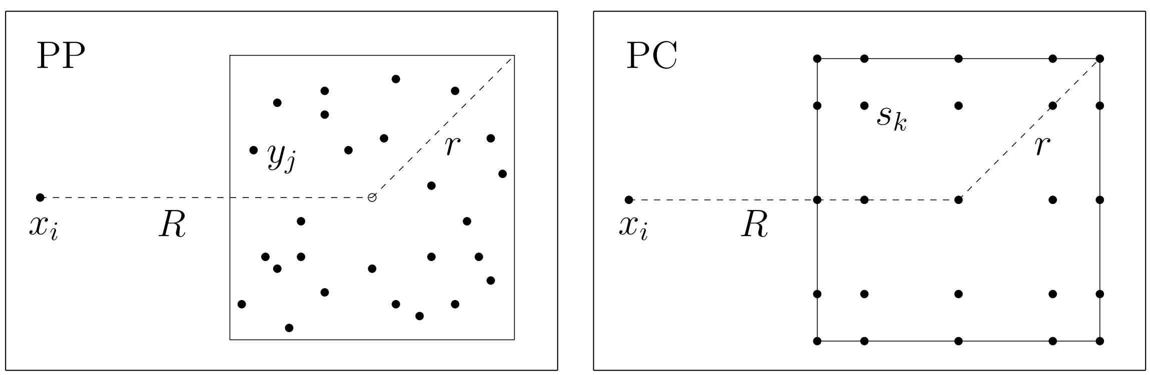
$s_k = (s_{k_1}, s_{k_2}, s_{k_3})$: Chebyshev points adapted to C

$$g(x,y) \approx \sum_{k_1=0}^{n} \sum_{k_2=0}^{n} \sum_{k_3=0}^{n} g(x, s_k) L_{k_1}(y_1) L_{k_2}(y_2) L_{k_3}(y_3)$$

- separated kernel approximation
- polynomial of degree n in y_1, y_2, y_3
- interpolates $g(x,y)$ at $y = s_k$
- accurate for $x \notin C$, $y \in C$
- kernel-independent

<u>BLTC</u> : barycentric Lagrange treecode (Wang-K-Tlupova 2020)

$$\phi_i = \sum_{j=1}^{N} g(x_i, y_j) q_j = \sum_{C} \sum_{y_j \in C} g(x_i, y_j) q_j \to \begin{cases} C_{\text{near}} : \text{particle-particle (PP)} \\ C_{\text{far}} : \text{particle-cluster (PC)} \end{cases}$$



$$\text{PP} : \sum_{y_j \in C} g(x_i, y_j) q_j$$

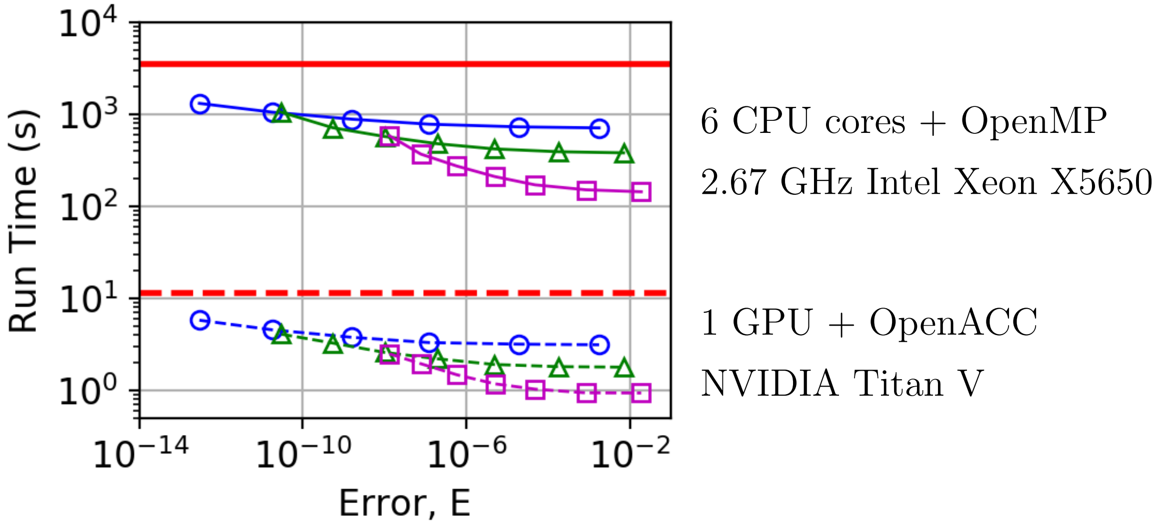
$$\text{PC} : \sum_{k_1=0}^{n} \sum_{k_2=0}^{n} \sum_{k_3=0}^{n} g(x_i, s_k) \widehat{q}_k \ , \ \widehat{q}_k = \sum_{y_j \in C} L_{k_1}(y_{j1}) L_{k_2}(y_{j2}) L_{k_3}(y_{j3}) q_j$$

1. PP and PC both have a direct sum form; the particles and charges (y_j, q_j) in PP are replaced by proxy particles and charges $(s_k, \widehat{q}_k)$ in PC.

2. use PC $\Leftrightarrow$ x_i , C are well-separated $\Leftrightarrow$ $r/R < \theta$: MAC

BLTC is well suited for GPU acceleration (Vaughn-Wilson-K 2020)

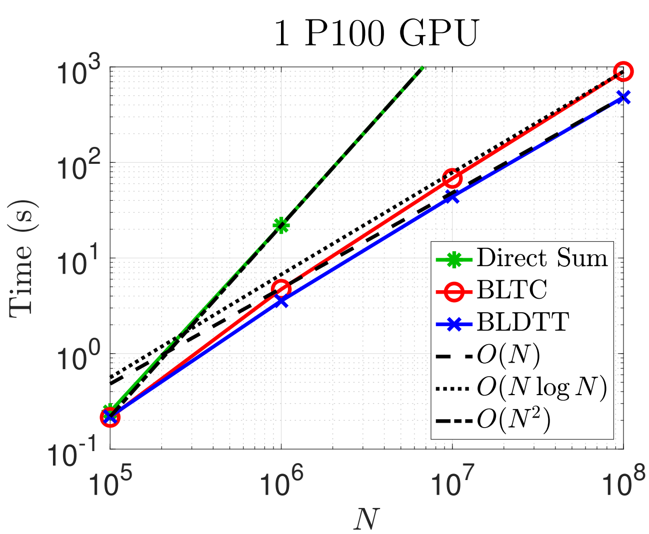
example : $N = 10^6$, $g(x, y) = |x - y|^{-1}$, $n = 1 : 2 : 13$, $\theta = 0.5, 0.7, 0.9$

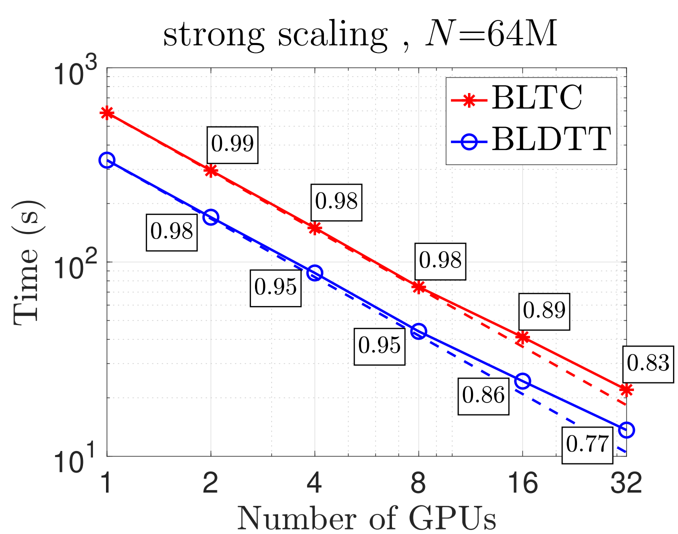


BLDTT = $O(N)$ (Wilson-Vaughn-K 2021)

- FMM upward/downward pass adapted to BLI
- interaction lists computed by dual tree traversal (Appel 1985)
- PP, PC, CP, CC

example : $g(x, y) = |x - y|^{-1}$, $n = 8$, $\theta = 0.7 \Rightarrow$ 7-8 digit accuracy

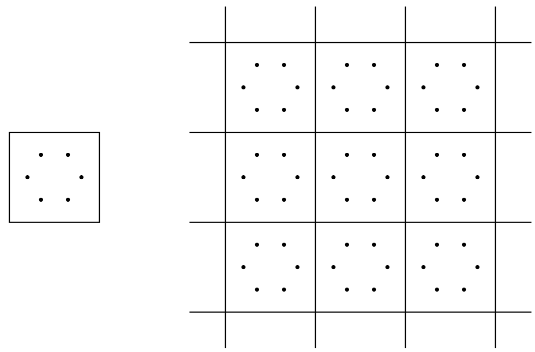




Codes are available at `https://github.com/Treecodes/BaryTree`.

periodic BC

Consider a set of charged particles in a cube, periodically repeated in $\mathbb{R}^3$.



$$V = \frac{1}{2} \sum_n {\sum_{i,j=1}^{N}}' \frac{q_i\, q_j}{4\pi |x_i - x_j + nL|}$$

L : cube side length

$n = (n_1, n_2, n_3)$, $n_i = 0, \pm 1, \ldots$

prime $\Rightarrow$ omit $i = j$ for $n = (0,0,0)$

1. V is the electrostatic potential energy due to interactions between charges in the central cell (x_i) and charges in the periodically repeated system ($x_j - nL$).
2. In computing V, a cutoff or the minimum image convention can be used for short-range interactions (e.g. Lennard-Jones), but this is not recommended for long-range interactions (e.g. Coulomb).

background on infinite series

1. $\sum_{n=1}^{\infty} a_n = \lim_{n\to\infty} \sum_{i=1}^{n} a_i$

If the limit of partial sums exists, then the series converges; otherwise, it diverges.

example : $\sum_{n=1}^{\infty} \frac{1}{2^n}$ converges , $\sum_{n=1}^{\infty} \frac{1}{n}$ diverges

2. A series $\sum_{n=1}^{\infty} a_n$ is absolutely convergent if $\sum_{n=1}^{\infty} |a_n|$ converges.

If $\sum_{n=1}^{\infty} a_n$ converges, but $\sum_{n=1}^{\infty} |a_n|$ diverges, then the series is conditionally convergent.

example : $\sum_{n=1}^{\infty} \frac{(-1)^n}{n^2}$ is absolutely convergent , $\sum_{n=1}^{\infty} \frac{(-1)^n}{n}$ is conditionally convergent

3. If a series is absolutely convergent, then reordering the terms does not change the sum, but if a series is conditionally convergent, then reordering the terms can change the sum.

example : $1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \frac{1}{5} - \frac{1}{6} + \frac{1}{7} - \frac{1}{8} + \cdots = \ln 2$: AHS

$$\frac{1}{2} - \frac{1}{4} + \frac{1}{6} - \frac{1}{8} + \frac{1}{10} - \frac{1}{12} + \frac{1}{14} - \frac{1}{16} + \cdots = \frac{1}{2}\ln 2$$

$$0 + \frac{1}{2} + 0 - \frac{1}{4} + 0 + \frac{1}{6} + 0 - \frac{1}{8} + \cdots = \frac{1}{2}\ln 2$$

$$1 + \frac{1}{3} - \frac{1}{2} + \frac{1}{5} + \frac{1}{7} - \frac{1}{4} + \frac{1}{9} + \frac{1}{11} - \cdots = \frac{3}{2}\ln 2 \text{ : reordered AHS}$$

We assume the central cell is charge neutral, i.e. $\sum_{i=1}^{N} q_i = 0$; this implies that the series for V is conditionally convergent; hence the sum depends on the order of summation, but regardless of the order chosen, the series converges slowly.

<u>Ewald summation</u> (Tosi 1964)

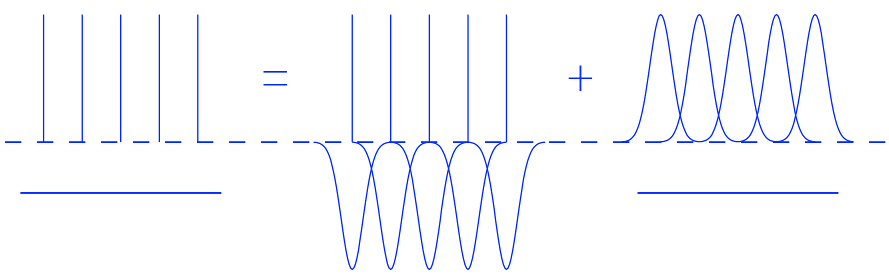
$\sum_n \frac{1}{4\pi|x+nL|}$: <u>lattice sum</u> , diverges for all x , but ok as a distribution

recall : $-\nabla^2 \frac{1}{4\pi|x|} = \delta(x) \Rightarrow -\nabla^2 \sum_n \frac{1}{4\pi|x+nL|} = \sum_n \delta(x+nL)$

set $\rho(x) = \sum_n \delta(x+nL) - \frac{1}{L^3}$, then $\int_{\text{cell}} \rho(x)dx = 0$: charge neutrality

Let $\psi(x)$ be the potential induced by $\rho(x)$, i.e. $-\nabla^2\psi = \rho$, with PBC. Then $\psi(x)$ is well-defined up to an additive constant; we will derive an efficient method for computing $\psi(x)$ and then use it to compute V.

$$\rho(x) = \left[\sum_n \big(\delta(x+nL) - f(x+nL)\big)\right] + \left[\sum_n f(x+nL) - \frac{1}{L^3}\right] = \rho_1(x) + \rho_2(x)$$



$f(x) = \frac{\alpha^3}{\pi^{3/2}} e^{-\alpha^2|x|^2}$: smooth , rapidly decaying , $\int_{\mathbb{R}^3} f(x)dx = 1$, pf ...

α^{-1} : Gaussian width , $\lim_{\alpha\to\infty} f(x) = \delta(x) \Rightarrow f(x)$: approximate delta-function

Let $\psi = \psi_1 + \psi_2$, where $-\nabla^2\psi_1 = \rho_1$, $-\nabla^2\psi_2 = \rho_2$, with PBC.

Then ψ_1, ψ_2 are well-defined up to additive constants by charge neutrality.

ρ : periodic sum of point charges + constant background

$\Rightarrow \psi$: no explicit expression other than $\psi_1 + \psi_2$

ρ_1 : periodic sum of screened point charges

$\Rightarrow \psi_1$: periodic sum of singular screened potentials, <u>decay rapidly in r</u>

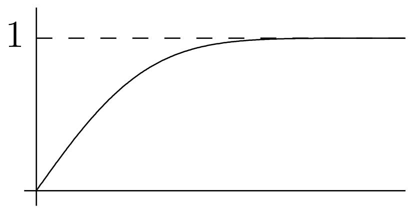
ρ_2 : periodic sum of smooth point charges + constant background

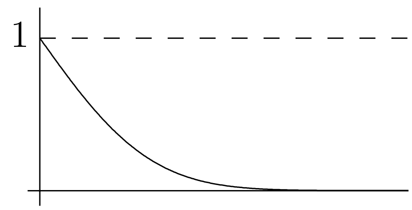
$\Rightarrow \psi_2$: periodic sum of smooth potentials, decay slowly in r, <u>decay rapidly in k</u>

claim

1. $\psi_1(x) = \sum_n \frac{\mathrm{erfc}(\alpha|x+nL|)}{4\pi|x+nL|} - \frac{1}{4\alpha^2 L^3}$

$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt$, $\mathrm{erfc}(x) = 1 - \mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-t^2}dt$





x	$\mathrm{erfc}(x)$
0	1.0000
1	0.1573
2	0.0047

2. $\psi_2(x) = \sum_{k\neq 0} \frac{\exp\left[-\frac{\pi^2|k|^2}{\alpha^2L^2} + 2\pi i k\cdot\frac{x}{L}\right]}{4\pi^2|k|^2 L}$: Fourier series , $\begin{cases} k = (k_1, k_2, k_3) \\ k_i = 0, \pm 1, \dots \end{cases}$

Hence $\psi_1(x)$, $\psi_2(x)$ are expressed as rapidly converging series.

1. $-\nabla^2\frac{\mathrm{erf}(\alpha|x|)}{4\pi|x|} = -\frac{1}{r^2}\partial_r\big(r^2\partial_r\big)\frac{\mathrm{erf}(\alpha r)}{4\pi r} = -\frac{1}{4\pi r^2}\partial_r\left[\cancel{r^2}\cdot\frac{r\cdot\frac{2}{\sqrt{\pi}}e^{-\alpha^2r^2}\cdot\alpha - \mathrm{erf}(\alpha r)}{\cancel{r^2}}\right]$

$= -\frac{1}{4\pi r^2}\left[r\cdot\frac{2}{\sqrt{\pi}}e^{-\alpha^2r^2}\cdot -2r\alpha^3 + \cancel{\frac{2}{\sqrt{\pi}}e^{-\alpha^2r^2}}\cdot\alpha - \cancel{\frac{2}{\sqrt{\pi}}e^{-\alpha^2r^2}}\cdot\alpha\right]$

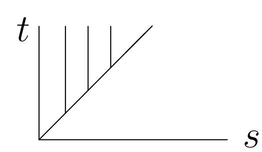
$= \frac{\alpha^3}{\pi^{3/2}}e^{-\alpha^2r^2} = f(x) \Rightarrow \frac{\mathrm{erf}(\alpha|x|)}{4\pi|x|}$: potential of a Gaussian charge density

$-\nabla^2\frac{\mathrm{erfc}(\alpha|x|)}{4\pi|x|} = -\nabla^2\frac{1-\mathrm{erf}(\alpha|x|)}{4\pi|x|} = \delta(x) - f(x) \ \Rightarrow \ \dots \ \Rightarrow \ -\nabla^2\psi_1 = \rho_1$

A constant is subtracted from $\psi_1(x)$ so that $\int_{\mathrm{cell}}\psi_1(x)dx = 0$.

$$\int_{\mathrm{cell}}\sum_n\frac{\mathrm{erfc}(\alpha|x+nL|)}{4\pi|x+nL|}\,dx = \int_{\mathbb{R}^3}\frac{\mathrm{erfc}(\alpha|x|)}{4\pi|x|}\,dx = \int_S\int_0^\infty\frac{\mathrm{erfc}(\alpha r)}{4\pi r}r^2drd\Omega \ , \ s = \alpha r$$

$$= \frac{1}{\alpha^2}\int_0^\infty \mathrm{erfc}(s)sds = \frac{1}{\alpha^2}\int_0^\infty\frac{2}{\sqrt{\pi}}\int_s^\infty e^{-t^2}dt\cdot sds$$



$$= \frac{1}{\alpha^2}\frac{2}{\sqrt{\pi}}\int_0^\infty e^{-t^2}\int_0^t s\,ds\,dt = \frac{1}{\alpha^2}\frac{\cancel{2}}{\sqrt{\pi}}\int_0^\infty e^{-t^2}\cdot\frac{t^2}{\cancel{2}}\,dt$$

$$= \frac{1}{\alpha^2}\frac{1}{\sqrt{\pi}}\left(\cancel{\frac{e^{-t^2}}{-2}\cdot t\Big|_0^\infty} - \int_0^\infty\frac{e^{-t^2}}{-2}dt\right) = \frac{1}{\alpha^2}\frac{1}{\sqrt{\pi}}\frac{1}{2}\frac{\sqrt{\pi}}{2} = \frac{1}{4\alpha^2} \quad \underline{\text{ok}}$$

2. $\rho_2(x) = \sum_k \widehat{\rho}_2(k)\, e^{2\pi i k \cdot x/L}$, $\widehat{\rho}_2(k) = \frac{1}{L^3}\int_{\text{cell}} \rho_2(x)\, e^{-2\pi i k \cdot x/L} dx$

$-\nabla^2 \psi_2 = \rho_2$, $\psi_2(x) = \sum_k \widehat{\psi}_2(k)\, e^{2\pi i k \cdot x/L} \Rightarrow \frac{4\pi^2|k|^2}{L^2}\, \widehat{\psi}_2(k) = \widehat{\rho}_2(k)$

$k = 0 \Rightarrow \widehat{\rho}_2(0) = \frac{1}{L^3}\int_{\text{cell}} \rho_2(x)\, dx = 0$: ok by charge neutrality

We choose $\widehat{\psi}_2(0) = 0$, so that $\int_{\text{cell}} \psi_2(x) dx = 0$.

now assume $k \neq 0$

$$\widehat{\rho}_2(k) = \frac{1}{L^3}\int_{\text{cell}} \left[\sum_n f(x+nL) - \cancel{\frac{1}{L^3}}\right] e^{-2\pi i k \cdot x/L} dx$$

$$= \frac{1}{L^3}\int_{\mathbb{R}^3} f(x) e^{-2\pi i k \cdot x/L} dx = \frac{1}{L^3}\int_{\mathbb{R}^3} \frac{\alpha^3}{\pi^{3/2}} e^{\left[-\alpha^2|x|^2 - 2\pi i k \cdot x/L\right]} dx$$

$$\int_{\mathbb{R}} e^{\left[-\alpha^2 x_1^2 \,-\, 2\pi i k_1 x_1/L\right]} dx_1 = \int_{\mathbb{R}} e^{\left[-\alpha^2\left(x_1 + \cancel{\frac{\pi i k_1}{\alpha^2 L}}\right)^2 - \frac{\pi^2 k_1^2}{\alpha^2 L^2}\right]} dx_1 \text{ , also } x_2, x_3$$

$$\widehat{\rho}_2(k) = \frac{1}{L^3}\frac{\alpha^3}{\pi^{3/2}}\, e^{-\frac{\pi^2|k|^2}{\alpha^2 L^2}} \left(\int_{\mathbb{R}} e^{-\alpha^2 x^2} dx\right)^3 = \frac{1}{L^3}\, e^{-\frac{\pi^2|k|^2}{\alpha^2 L^2}} \qquad \underline{\text{ok}}$$

<u>summary of lattice sum</u>

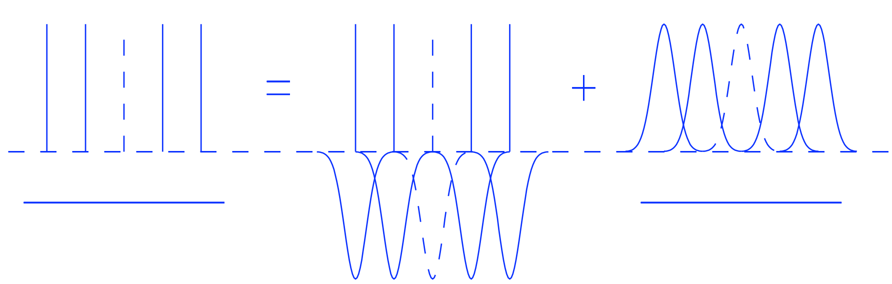
$$\rho(x) = \sum_n \delta(x+nL) - \frac{1}{L^3}$$

$$\psi(x) = \sum_n \frac{\operatorname{erfc}(\alpha|x+nL|)}{4\pi|x+nL|} - \frac{1}{4\alpha^2 L^3} + \sum_{k\neq 0} \frac{\exp\left[\frac{-\pi^2|k|^2}{\alpha^2 L^2} + 2\pi i k \cdot \frac{x}{L}\right]}{4\pi^2|k|^2 L}$$

In evaluating V, there are two types of terms.

1. $i \neq j$: use $\psi(x)$ with $x = x_i - x_j$
2. $i = j$: use $\psi(x)$ with $x = x_i - x_j = 0$, but omit $n = 0$ term

in this case consider $\widetilde{\rho}(x) = \rho(x) - \delta(x) = [\rho_1(x) - \delta(x) + f(x)] + [\rho_2(x) - f(x)]$



$$\widetilde{\psi}(x) = \sum_{n\neq 0} \frac{\operatorname{erfc}(\alpha|x+nL|)}{4\pi|x+nL|} - \frac{1}{4\alpha^2L^3} + \sum_{k\neq 0} \frac{\exp\left[-\dfrac{\pi^2|k|^2}{\alpha^2L^2} + 2\pi ik\cdot\dfrac{x}{L}\right]}{4\pi^2|k|^2L} - \frac{\operatorname{erf}(\alpha|x|)}{4\pi|x|}$$

$$\widetilde{\psi}(0) = \sum_{n\neq 0} \frac{\operatorname{erfc}(\alpha|nL|)}{4\pi|nL|} - \frac{1}{4\alpha^2L^3} + \sum_{k\neq 0} \frac{\exp\left[-\dfrac{\pi^2|k|^2}{\alpha^2L^2}\right]}{4\pi^2|k|^2L} - \frac{1}{4\pi}\frac{2}{\sqrt{\pi}}\alpha$$

$\widetilde{\psi}(0)$ is the self-potential at a charge due to its periodic images.

$$V = \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N} q_iq_j\psi(x_i-x_j) + \frac{1}{2}\sum_{i=1}^{N} q_i^2\widetilde{\psi}(0) = V^r + V^k + V^s \ :\ \text{Ewald summation}$$

$$V^r = \frac{1}{2}\sum_{n}\sum_{i,j=1}^{N}{}' q_iq_j \frac{\operatorname{erfc}(\alpha|x_i-x_j+nL|)}{4\pi|x_i-x_j+nL|} \ :\ \text{real-space term}$$

$$V^k = \frac{1}{2}\sum_{i,j=1}^{N} q_iq_j \sum_{k\neq 0} \frac{\exp\left[-\dfrac{\pi^2|k|^2}{\alpha^2L^2} + 2\pi ik\cdot\dfrac{x_i-x_j}{L}\right]}{4\pi^2|k|^2L} \ :\ \text{reciprocal-space term}$$

$$V^s = \frac{-\alpha}{4\pi^{3/2}}\sum_{i=1}^{N} q_i^2 \ :\ \text{self-energy term}$$

1. The terms involving $\dfrac{1}{4\alpha^2L^3}$ drop out by charge neutrality.

2. The expression for V is an identity for all $\alpha > 0$.

3. V^r, V^k are rapidly converging sums that can be evaluated using cutoffs, $|x_i - x_j + nL| < r_c, |k| \leq k_c$.

$$\text{large } \alpha \Rightarrow \begin{cases} V^r \text{ converges rapidly} : O(N) \\ V^k \text{ converges slowly} : O(N^2) \end{cases}$$

$$\text{small } \alpha \Rightarrow \begin{cases} V^r \text{ converges slowly} : O(N^2) \\ V^k \text{ converges rapidly} : O(N) \end{cases}$$

4. By choosing α, r_c, k_c properly, the cost can be reduced to $O(N^{3/2})$.

5. For large α, the cost of computing V^k can be reduced to $O(N\log N)$ using the FFT-based particle-mesh Ewald method (Darden-York-Pedersen 1993).

6. For small α, the cost of computing V^r can be reduced to $O(N\log N)$ using a treecode (Duan-K 2000) or to $O(N)$ using BLDTT (Wilson-Vaughn-K 2021).