Velocity Autocorrelation Function

2/13/92

$$Z_\alpha(t) = \left\langle \sum_{i=1}^{N_\alpha} \vec{V}_i(t+t_0)\cdot\vec{V}_i(t_0)\right\rangle \Big/ \left\langle \sum_{i=1}^{N_\alpha} |\vec{V}_i(t_0)|^2 \right\rangle \qquad (1)$$

where α = Si or O.

(Symmetry)

$$Z_\alpha(t) = Z_\alpha(-t) \qquad (2)$$

$$\because\ Z_\alpha(-t)\left\langle \sum_{i=1}^{N_\alpha} |\vec{V}_i(t_0)|^2\right\rangle = \left\langle \sum_{i=1}^{N_\alpha} \vec{V}_i(-t+t_0)\cdot\vec{V}_i(t_0)\right\rangle$$

$$= \left\langle \sum_{i=1}^{N_\alpha} \vec{V}_i(t_0)\cdot\vec{V}_i(-t+t_0)\right\rangle$$

+t; time invariance

$$= \left\langle \sum_{i=1}^{N_\alpha} \vec{V}_i(t-t_0)\cdot\vec{V}_i(t_0)\right\rangle$$

$$= Z_\alpha(t)\left\langle \sum_{i=1}^{N_\alpha} |\vec{V}_i(t_0)|^2\right\rangle \qquad //$$

§. Power Spectrum

$$G_\alpha(\omega) \equiv \frac{3N_\alpha}{\pi}\int_{-\infty}^{\infty} dt\, Z_\alpha(t)\, e^{i\omega t} \qquad (3)$$

$$= \frac{6N_\alpha}{\pi}\int_0^{\infty} dt\, Z_\alpha(t)\cos\omega t \qquad (4)$$

$\because$ Eqs. (3) = (4)

$$\text{Eq. (3)} = \frac{3N_\alpha}{\pi}\Big(\underbrace{\int_{-\infty}^{0} dt\, Z_\alpha(t)\, e^{i\omega t}}_{t\leftrightarrow -t} + \int_0^{\infty} dt\, Z_\alpha(t)\, e^{i\omega t} \Big)$$

$$= \int_0^{\infty} dt\, \underbrace{Z_\alpha(-t)}_{Z_\alpha(t)\ (\because \text{Eq.}(2))} e^{-i\omega t}$$

$$= \frac{3N_\alpha}{\pi}\int_0^{\infty} dt\, Z_\alpha(t)\, \underbrace{(e^{i\omega t}+e^{-i\omega t})}_{2\cos\omega t} \qquad //$$

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(Symmetry)

$$G_\alpha(-\omega) = G_\alpha(\omega) \tag{5}$$

$\because$

$$G_\alpha(-\omega) = \underbrace{\frac{3N_\alpha}{\pi}\int_{-\infty}^{\infty} dt\, Z_\alpha(t)\, e^{-i\omega t}}_{t \leftrightarrow -t} = G_\alpha(\omega)$$

$$= \int_{-\infty}^{\infty} dt\, \underbrace{Z_\alpha(-t)}_{Z_\alpha(t)\ (\because \text{Eq.}(2))}\, e^{i\omega t}$$

//

(Normalization)

$$\int_0^\infty d\omega\, G_\alpha(\omega) = \frac{1}{2}\int_{-\infty}^{\infty} d\omega\, G_\alpha(\omega) \quad (\because \text{Eq.}(5))$$

$$= \frac{1}{\cancel{2}} \int_{-\infty}^{\infty} d\omega\, \frac{3N_\alpha}{\cancel{\pi}} \int_{-\infty}^{\infty} Z_\alpha(t)\, e^{i\omega t}\, dt$$

$$\to \cancel{2\pi}\,\delta(t)$$

$$= 3N_\alpha\, \underbrace{Z_\alpha(0)}_{=1}$$ from the definition

$$\therefore \int_0^\infty d\omega\, G_\alpha(\omega) = 3N_\alpha \tag{6}$$

(Total Power Spectrum)

$$G(\omega) = \sum_\alpha G_\alpha(\omega) \tag{7}$$

so that

$$\int_0^\infty d\omega\, G(\omega) = 3N \tag{8}$$

§. Program

Since the normalization factor is just to make $Z_\alpha(0) = 0$, we define

we can use $\vec{X}_1$ instead of $\vec{V}$

$$Z'_\alpha(t) = \Delta t^2 \left\langle \sum_{i=1}^{N_\alpha} \vec{V}_i(t+t_0) \cdot \vec{V}_i(t_0) \right\rangle , \qquad (9)$$

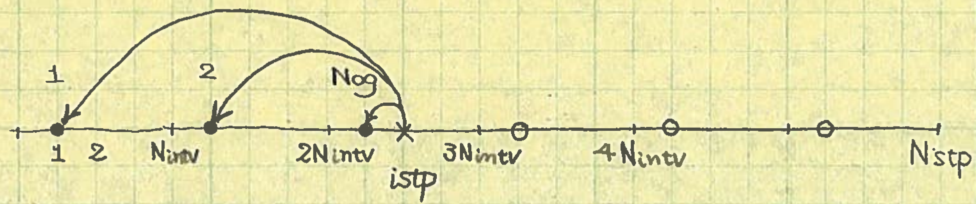
and at the end of a program,

$$Z_\alpha(t) = Z'_\alpha(t) \,/\, Z'_\alpha(0) \qquad (10)$$

$\rightarrow$ Δt^2 doesn't appear.

(Time Average)

$$Z'_\alpha(t) = \frac{1}{N_{sample}} \sum_{t_0=1}^{N_{sample}} \left[\sum_{i=1}^{N_\alpha} \vec{V}_i(t+t_0) \cdot \vec{V}_i(t_0) \right] \qquad (11)$$



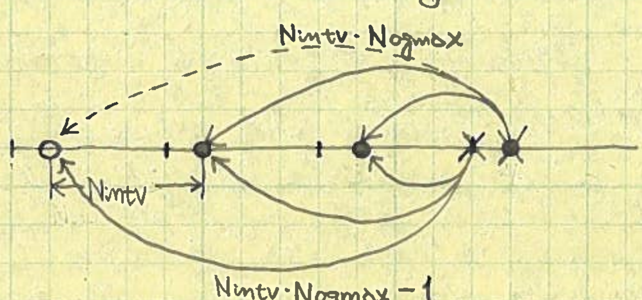
Every N_{intv} steps, we store velocities as time origins. N_{og} (variable) is the # of time origins stored by the current step, $istp$. Only the last N_{ogmax} origins are kept in memory. N_{cormax} is the maximum time steps for the velocity autocorrelation function.

$$\begin{cases} ZA(\emptyset : N_{cormax}, N_c) & \leftarrow \quad Z_\alpha(t) \\ V\emptyset(N_{max3}, N_{ogmax}) & \leftarrow \quad \vec{v}_i(t_0) \text{ for the last } N_{ogmax}\ t_0\text{'s} \\ NORM(\emptyset : N_{cormax}) & \leftarrow \quad \text{\# of samples of correlations} \end{cases}$$

We set

$$N_{cormax} = N_{intv} \cdot N_{ogmax} - 1 \tag{12}$$

☹ Suppose $N_{intv} = 4$ and $N_{ogmax} = 3$



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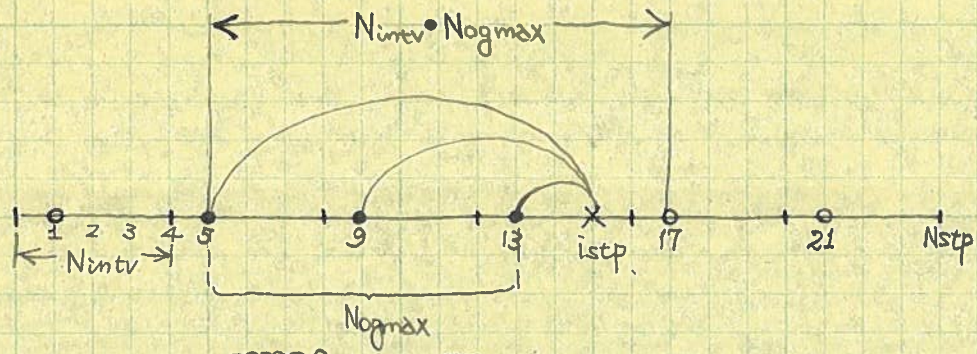
(Data Organization of VØ)



istp	Nog	ISTPOG 1	ISTPOG 2	ISTPOG Nogmax	NOG 1	NOG 2	NOG Nogmax
1	1	1	Ø	Ø	1	X	X
5	2	1	5	Ø	1	2	X
9	3	1	5	9	1	2	3
13	4	13	5	9	4	2	3
17	5	13	17	9	4	5	3
21	6	13	17	21	4	5	6

ISTPOG(NOGMAX) ← Time step of the origins

(Argorithm)

** Initialization **

$$\begin{cases} Nog = \emptyset \\ Norm(i) = 0 \quad (i = 0, Ncormax) \\ Istpog(j) = 0 \quad (j = 1, Nogmax) \end{cases}$$

** Sampling **

```
do  istp = 1,  Nstp
    if ( mod(istp, Nintv) = 1 )  then
        Nog = Nog + 1
        j = mod(Nog, Nogmax)
         if (j ≤ 0)  j = Nogmax
        Istpog(j) = istp
        V̇φ(i,j) = X1(i)    (i = 1,3N)
    endif

    do  j = 1,  Nogmax
        if ( Istpog(j) = 0 )  goto  enddo
        idt = istp - Istpog(j)
        if (idt ≤ Ncormax)   then
            Norm(idt) = Norm(idt) + 1
```

$$Z(idt, \alpha) = Z(idt, \alpha) + \sum_{i=1}^{N} \vec{X}_1(i) \cdot \vec{\dot{V}}\phi(i,j)\, \delta_{i_S(i),\alpha}$$

```
        endif
    enddo

enddo
```

** BAMOVE **

Don't forget to move $\vec{V}_\phi$ together with $\vec{X}_1$.

** Final processing **

```
do  i = Ø, Ncormax
    ZA(i,α) = ZA(i,α) / Norm(i)     (α=1, Nmass)
enddo
do  i = Ncormax, Ø, -1
    ZA(i,α) = ZA(i,α) / ZA(Ø,α)  (α=1, Nmass)
enddo
```

** DOS **

GA($N_{\omega max}$, Nmass) $\leftarrow$ $G_\alpha(\omega)$

Wmin, Wmax, TAUDOS

$$G_\alpha(\omega) = \frac{6N\alpha}{\pi} \Delta t \sum_{i=0}^{N_{cormax}} Z_\alpha(t_i) \cos(\omega t_i)\, e^{-(t_i/\tau_{dos})^2}$$