HIERARCHICAL PCA HPCA
STEPI CONSTRUCT SECTIONS
> SECTION 1) N
SECTION 2 NON
SECTION 3 OVERLAPINE
SECTIONS
PROTEIN SECTION N)
Structure SECTION N+1) m
SECTION N+2 S SPECIAL
\$ SEctions
SECCION N+M}
WhoLE PROCEIN N+m+1
 STEP 2 RUN JED ON ALL SECTIONS
TAKE TOP 5 PCA 1700ES
NOTE: CAN BE SPECIFIED
BY USER BASED ON
SCREE PLOTS, Etc.
JERCE FLOOR, EC-
 STEP3 CONSTRUCT INPUT FILE
JED-ANALYSIS
RUN MATLAB INPUT FILE)
SECTION 1 SECTION N+M+1
JED2 HPCA

	RESULTS FROM JEDZHPCA
	JED-ANALYSIS
	PROTEIN SYSTEM P1 P2 P3 111/ PN COMPARATIVE-AVALYSIS JED-ANALYSIS JED-ANALYSIS OUTPUT TYPES DIFFERENT OUTPUT TYPES
	T00L5}
*-	MATHMATICS OF HPCA K-th LET J:S,K = CPCA MODE FOR SECTIONS COVARIANCE MATRIX ** ORDERING OF OVERLAPPING SECTIONS IS IMPORTANT, BEST TO POT SMALLEST -> LARGEST MOST NON-OVERLAPPING BEFORE OVERLAPPING
	DEFINE LINEAR INDEX IN 6 SCHEME EXAMPLE 9 SECTIONS EACH WITH 5 MODES. 1 2 3 4 5 6 7 8 9 10 11 44 45 1,1 1,2 1,3 1,4 1,5 2,1 2,2 2,3 2,4 2,5 3,1 9,4 9,5 MAP $n \leftrightarrow \{s,F\}_n$ APPLY PROJECTION OPERATOR METHOD

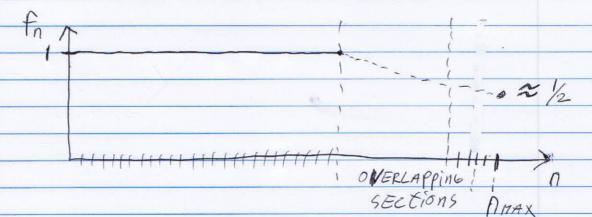
$$|V_{i}\rangle \equiv |J_{i}|_{i}|_{i}$$

$$DEFINE P_{i} \equiv 1 = \sum_{k=1}^{n} |V_{k}\rangle \langle V_{k}|_{i}$$

itERATIVELY SOLVE:

$$|V_{n+1}\rangle = \hat{P}_n |\mathcal{T}: \{5, K\}_{n+1}\rangle$$

MOVITOR OVERLAPS:



EACH | Vn+1) MONITORS AN ORTHOGONAL

type of motion to the set & [VK] TE=1,11

Note: NON-OVER LAPPING SEctions

OVER LAPPING SECTIONS -O Section o J: 5, K, gection o-J:52, K2 < J: 52, K2 J: S, K) = O in GENERAL $\langle V_{02} | V_{0} \rangle = 0$ ALWAYS. where n => {5, 16, } n => {5, 162} BUILD COVARIANCE AND CORRELATION MATRICES GENERALIZED INTERNAL COOR dinAtES: { In(t)} $g_n(t) = \langle v_n | C(t) \rangle$ | c(t) > = conformation of protein time frame of other indexing X, Y, Z COMPONENTS ARE BEING TRACKED! NEXT CONSTRUCT M CORRELATION EIGENVALUES / EIGENVECTORS OF M { 2, 10,>} CAN LOOK @ innER PRODUCTS <Un /Un> COLLAPSED innER PRODUCTS-5 (Us | Us) COMBINED iNNER PRODUCTS

OUTER PRODUCTS & Un> 2, < Un| CONSTRUCT Pn = S < K | Un > 1 VK Note |Un> = E < K Un> (K) K L COMPONENTS OF the O-th EiGEN VECTOR Note: $\langle \rho_m | \rho_n \rangle = \sum_{j \in K} \langle v_j | \langle v_m | j \rangle \langle k | v_n \rangle | V_k \rangle$ (Vi VK) = SiK $\langle Q_m | Q_n \rangle = \sum_{k} \langle Q_n | k \rangle \langle k | Q_n \rangle$ $\sum_{k} | \langle Q_n | k \rangle \langle k | Q_n \rangle$ $\langle Q_m | Q_n \rangle = \langle U | U_n \rangle = S_{mn}$ S(Qn) = ORTOGONAL SET OF MODES