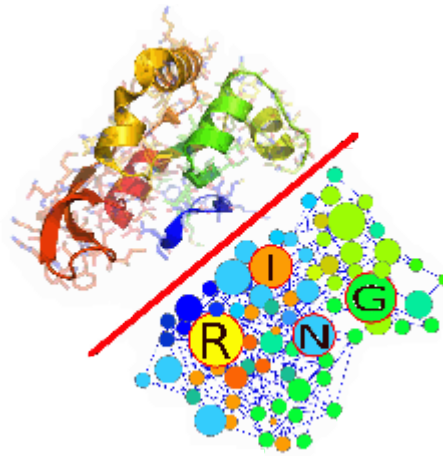


RING

Residue Interaction Network Generator



Contatti

Università di Padova - Dipartimento di biologia medica

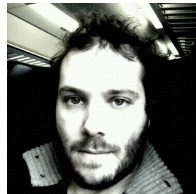
Laboratorio Biocomputing

<http://protein.bio.unipd.it/>



Silvio Tosatto

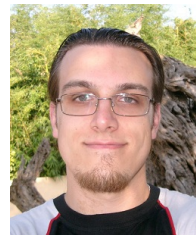
Group Leader



Damiano Piovesan

Postdoc

damianopiovesan@gmail.com



Manuel Giollo

Dottorando

manuel.giollo@gmail.com

A metà novembre terremo dei **seminari introduttivi!**

Bioinformatics

“The study of information processes in biological systems”

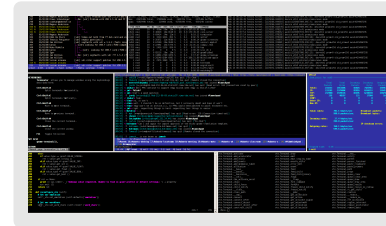
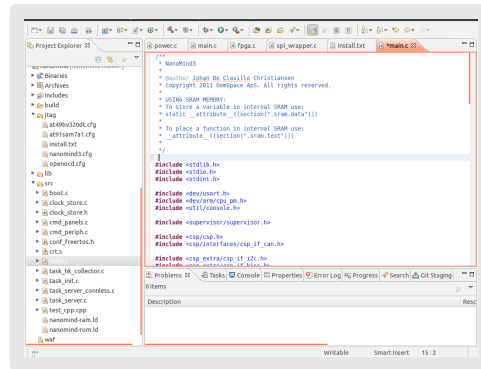
Paulien Hogeweg, 1970

...ma anche....

Sviluppo di tools per
rendere la vita facile ai
biologi!



Il “Dogma” della Biologia Molecolare

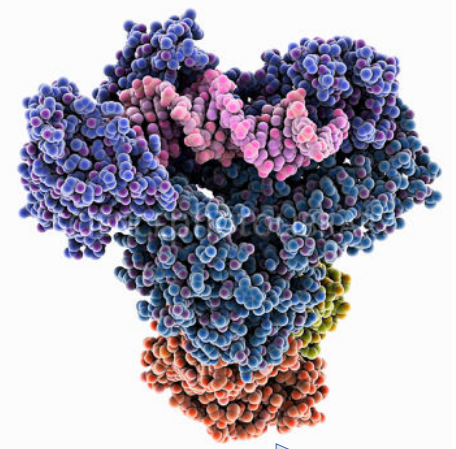
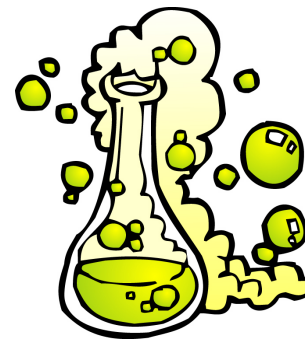
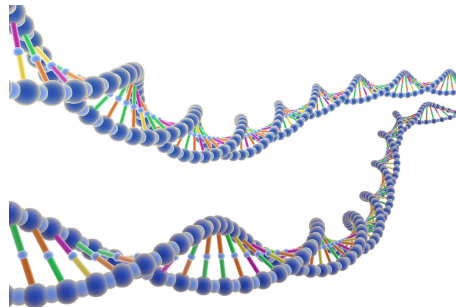


Creatore

Codice sorgente

Compilazione

Programma



Creatore

Gene

Biochimica

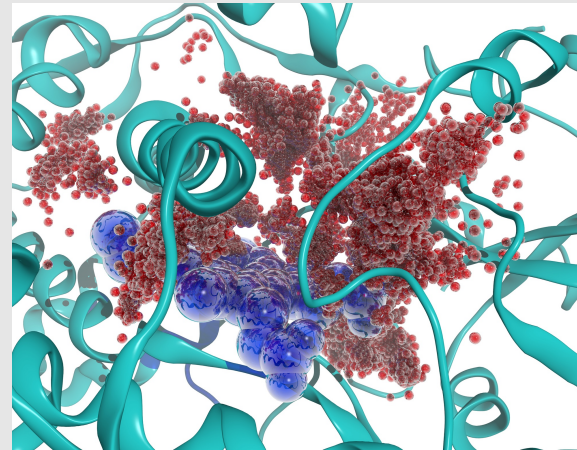
Proteina

Le proteine fanno cose...



DNA Learning Center (<http://www.dnalc.org>)

La funzionalità delle proteine dipende dalla loro struttura



Citocromo P450

Detossificazione di farmaci e tossine. Se l'acqua (rosso) non raggiunge il **sito attivo** (blu) la proteina non funziona.

No Struttura



No Funzione



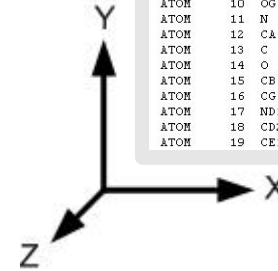
Malattia

Determinazione delle strutture proteiche



Scienziati

ATOM	1	N	GLY	A	1	44.842	51.034	101.284	0.01	27.20
ATOM	2	CA	GLY	A	1	45.640	50.230	100.389	0.01	26.99
ATOM	3	C	GLY	A	1	46.692	49.648	101.308	0.01	26.80
ATOM	4	O	GLY	A	1	46.895	50.222	102.381	0.01	26.91
ATOM	5	N	SER	A	2	47.283	48.516	100.951	1.00	26.26
ATOM	6	CA	SER	A	2	48.277	47.866	101.761	1.00	26.17
ATOM	7	C	SER	A	2	49.212	47.031	100.845	1.00	24.21
ATOM	8	O	SER	A	2	49.060	47.195	99.630	1.00	19.77
ATOM	9	CB	SER	A	2	47.438	47.091	102.800	1.00	26.31
ATOM	10	OG	SER	A	2	46.276	46.356	102.404	1.00	27.99
ATOM	11	N	HIS	A	3	50.147	46.186	101.370	1.00	23.93
ATOM	12	CA	HIS	A	3	51.129	45.389	100.609	1.00	21.44
ATOM	13	C	HIS	A	3	50.953	43.905	100.849	1.00	20.32
ATOM	14	O	HIS	A	3	50.530	43.595	101.950	1.00	22.00
ATOM	15	CB	HIS	A	3	52.555	45.674	100.990	1.00	19.69
ATOM	16	CG	HIS	A	3	52.940	47.090	100.611	1.00	21.44
ATOM	17	ND1	HIS	A	3	53.371	47.470	99.422	1.00	20.87
ATOM	18	CD2	HIS	A	3	52.956	48.175	101.433	1.00	21.69
ATOM	19	CE1	HIS	A	3	53.676	48.730	99.476	1.00	20.57



Coordinate 3D

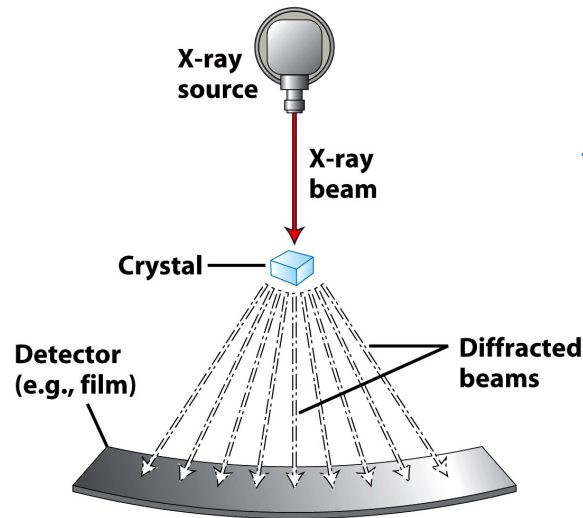


Figure 3-42a
Molecular Cell Biology, Sixth Edition
© 2008 W.H. Freeman and Company

Esperimenti

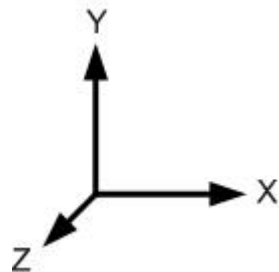
RCSB **PDB**
PROTEIN DATA BANK



Studio delle strutture

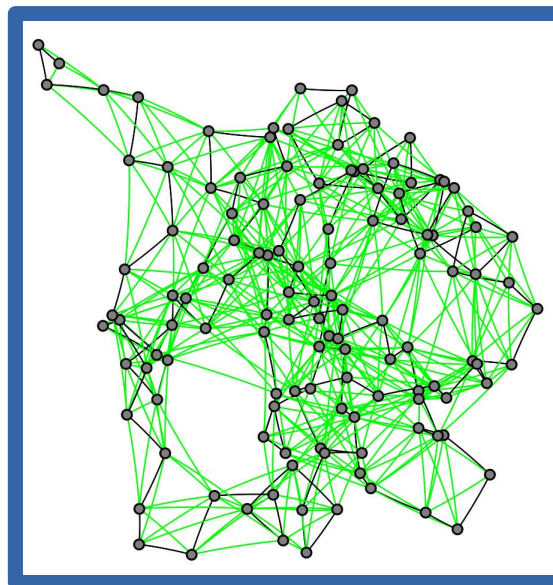
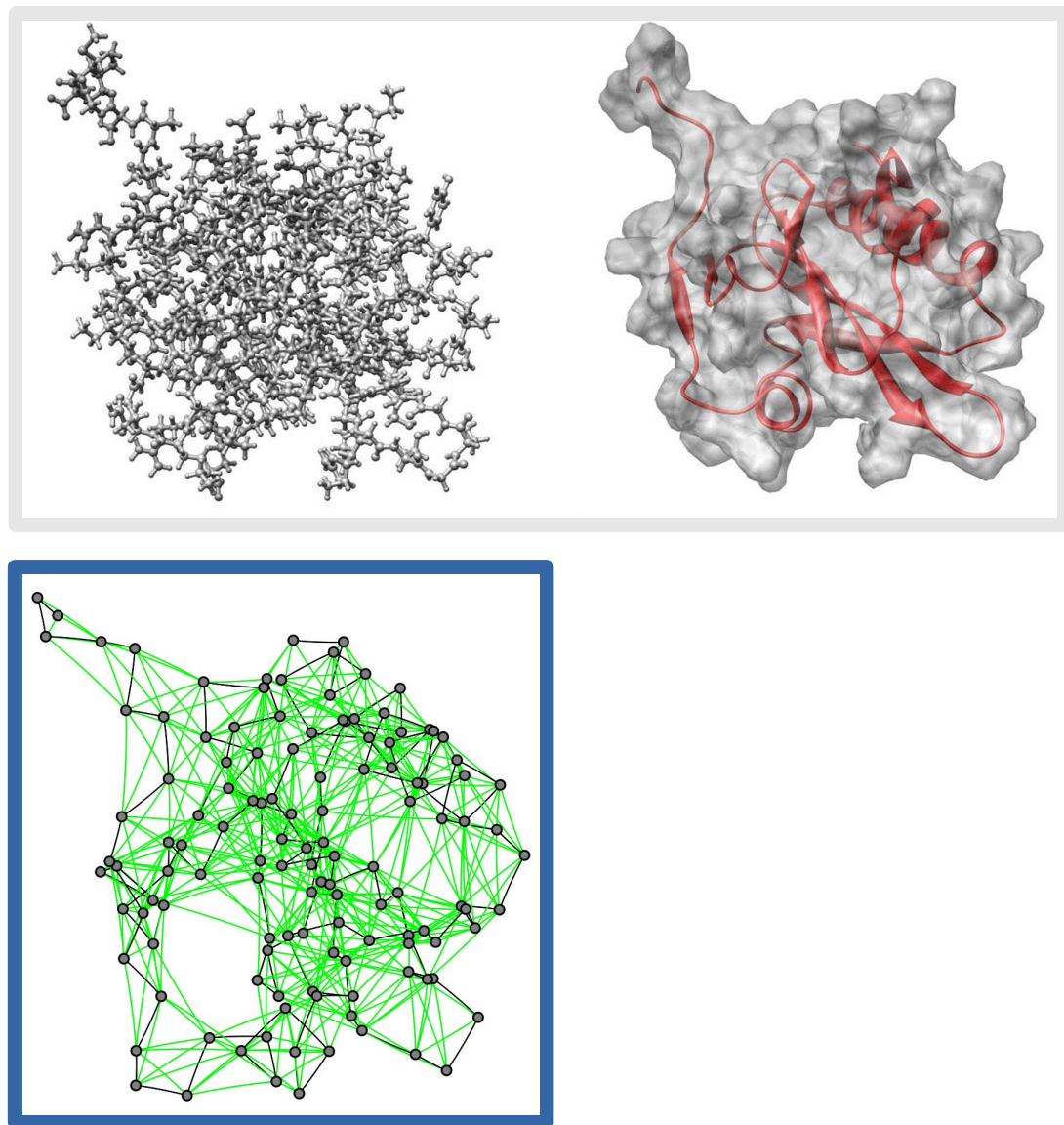
Coordinate

ATOM	1	N	GLY	A	1	44.842	51.034	101.284	0.01	27.20
ATOM	2	CA	GLY	A	1	45.640	50.230	100.389	0.01	26.99
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ATOM	6	CA	SER	A	2	48.277	47.866	101.761	1.00	26.17
ATOM	7	C	SER	A	2	49.212	47.031	100.845	1.00	24.21
ATOM	8	O	SER	A	2	49.060	47.195	99.630	1.00	19.77
ATOM	9	CB	SER	A	2	47.438	47.091	102.800	1.00	26.31
ATOM	10	OG	SER	A	2	46.276	46.356	102.404	1.00	27.99
ATOM	11	N	HIS	A	3	50.147	46.186	101.370	1.00	23.93
ATOM	12	CA	HIS	A	3	51.129	45.389	100.609	1.00	21.44
ATOM	13	C	HIS	A	3	50.953	43.905	100.849	1.00	20.32
ATOM	14	O	HIS	A	3	50.530	43.595	101.950	1.00	22.00
ATOM	15	CB	HIS	A	3	52.555	45.674	100.990	1.00	19.69
ATOM	16	CG	HIS	A	3	52.940	47.090	100.611	1.00	21.44
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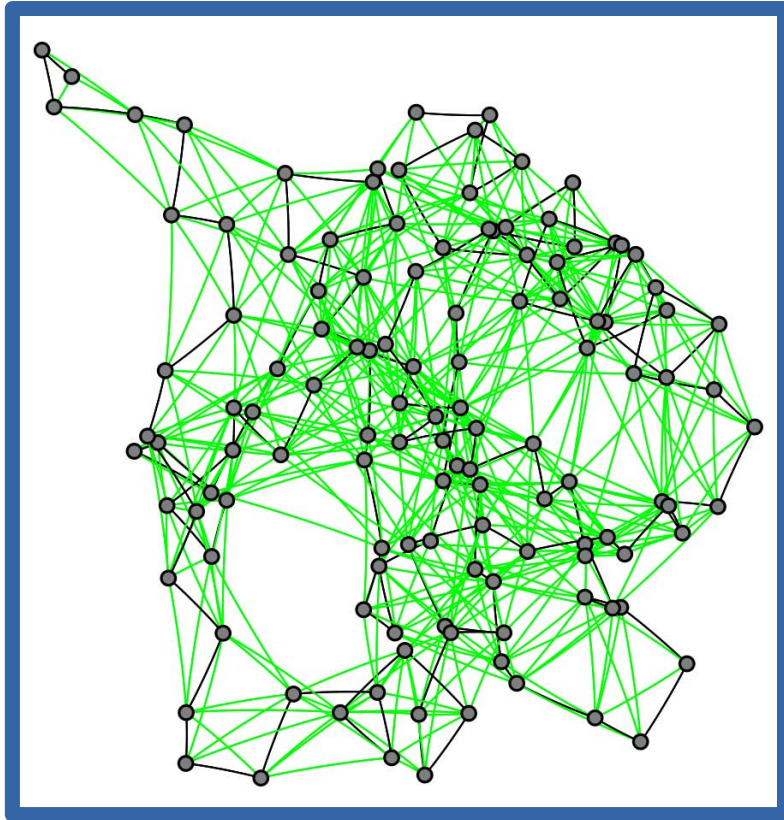


RASMOL

RING



Residue Interaction Network (RIN)



Nodo Atomo

Arco Interazione tra 2 atomi (vicinanza spaziale)

Attributi archi Tipo di legame (covalente, idrogeno, etc...)

Attributi nodi Tipo di atomo, carica, conservazione, etc...

Numero di nodi $400 < x < 500K$ (media 3K)

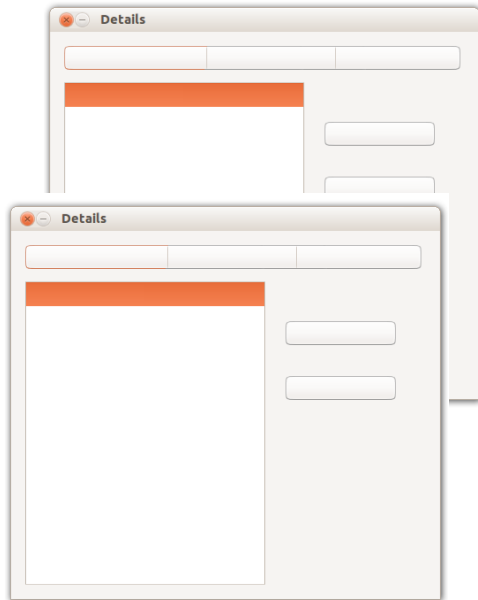
RING – Requisiti (1/3)

*Analisi e
visualizzazione reti*



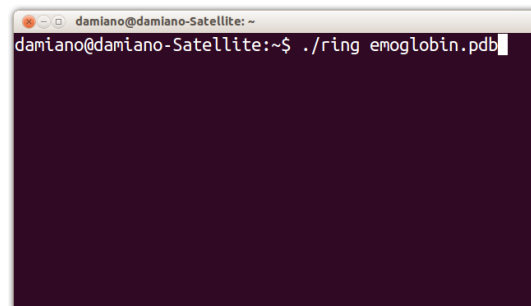
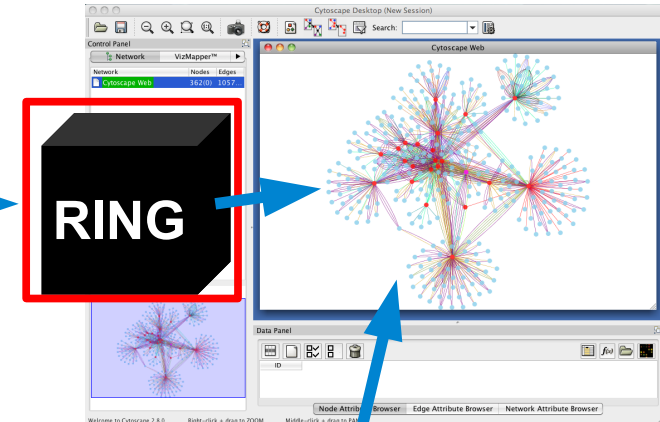
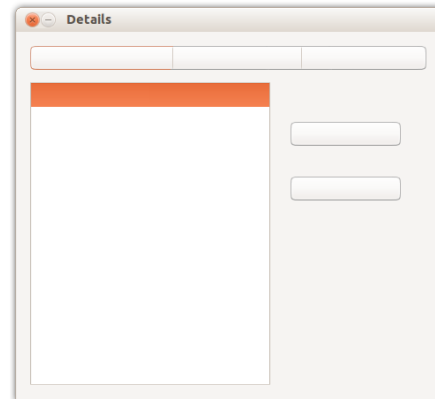
RING – Requisiti (2/3)

Carica (1 PDB)



Edita RIN
(aggiungi attributi)

Carica MD (100K PDB)



RING – Requisiti (3/3)

Velocità **1 rete** calcolata in pochi **secondi**

Parallelizzazione **N reti** calcolate utilizzando un numero di **thread** deciso dall'utente (in modalità command line)

Documentazione **Manuale** utente, documentazione del codice (**Doxygen** o **Javadoc**)

Linguaggio **C++** o **Java**

Thanks!