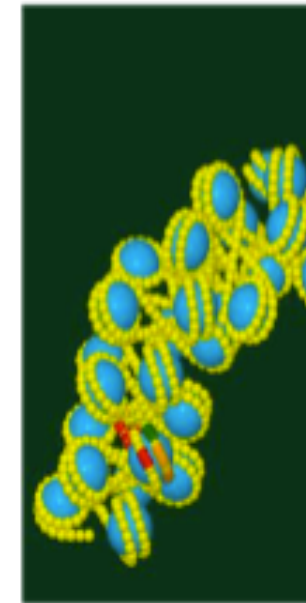
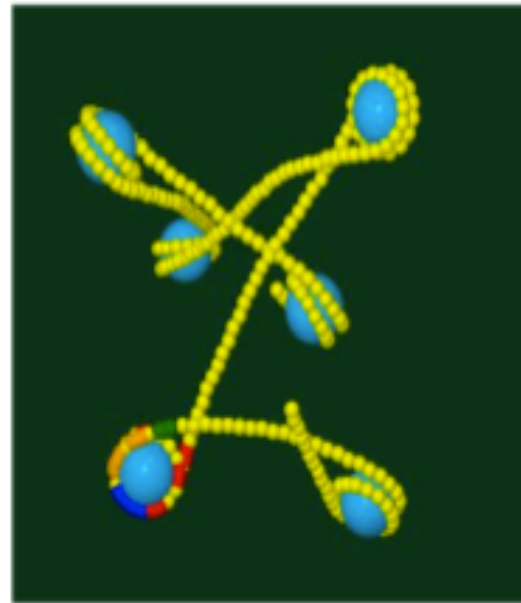
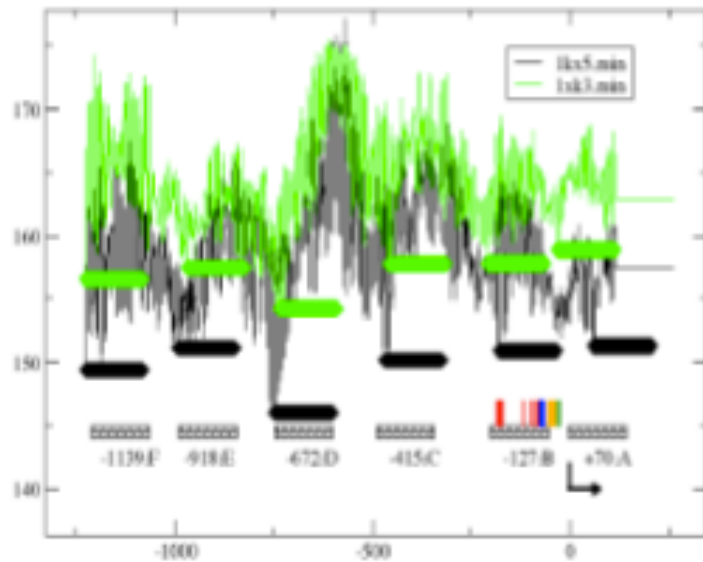


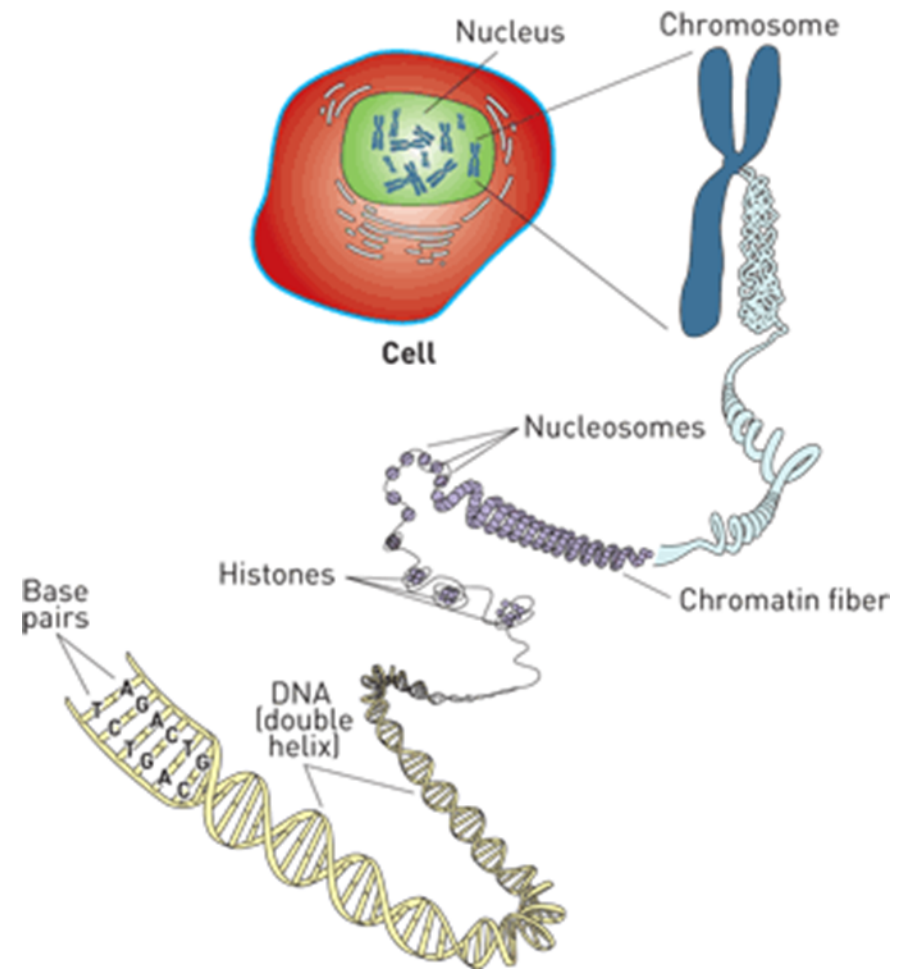
Developing the Interactive Chromatin Modeling Program



John Bell
Southern University at Shreveport

ICM

- What is chromatin?



Chem. & Eng. News;
July 17, 2006

ICM

What is Interactive Chromatin Modeling (ICM)

- Integration of bioinformatics and computational biology
- Graphic representation

ICM-Web

www.LaTech.edu/~bishop, click the tab
“Chromatin Folding”

Interactive Chromatin Modeling
ICM ~ I see 'em
details
Nucleic Acids Res. 2010 38:W254-W261.
DOI:10.1093/nar/gkq496

Sequence Input Options:
 Default Sequence Type Sequence Upload Sequence
This option allows for sequence input.
Please insert your sequence:
Type or cut-and-paste sequence here.
Try one of our samples below or search PubMed
SS_dimer

Thermal Fluctuation:
This option controls the level of thermal fluctuation.
Temperature: 298 Kelvin

Nucleosome Placement Options:
 Use Default Parameters Use Energy Calculations Specify Nucleosome Placement
These options control automatic placement of nucleosomes in the energy landscape.

Energy Options:
 $E_{nuc} = \frac{1}{2} \sum (K(X_{nuc} - X_{DNA})^2)$
K = MD-B.dat
X_{nuc} = 01kx5_min
X_{DNA} = MD-B.par

Occupancy:
Occupancy: .70
Linker Length: 20

Go Reset

[Click here for References](#) [Click here for Related Sites](#)

Home	Background	Contact	Publications	Research	Calendar
Classes	Lab	Chromatin Folding	DNA Maker	VDNA	ManyJobs

Reset Larger Window

Reset Larger Window

Yellow = 5bp DNA bead.
First 5bp bead is green.
Blue = histone core.
Red indicates close contact.

Close Contacts:
Nuc-Nuc: 241(Å): None
Nuc-DNA: 92(Å): None
DNA-DNA: 12(Å): Contact

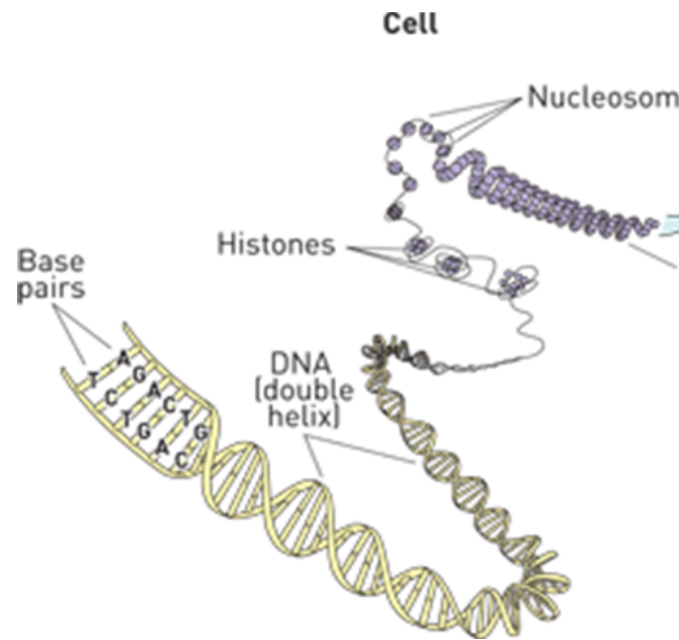
Nucleosome Energy Level Diagram

Energy (kcal/mol)

Energy Index

ICM – Parameters

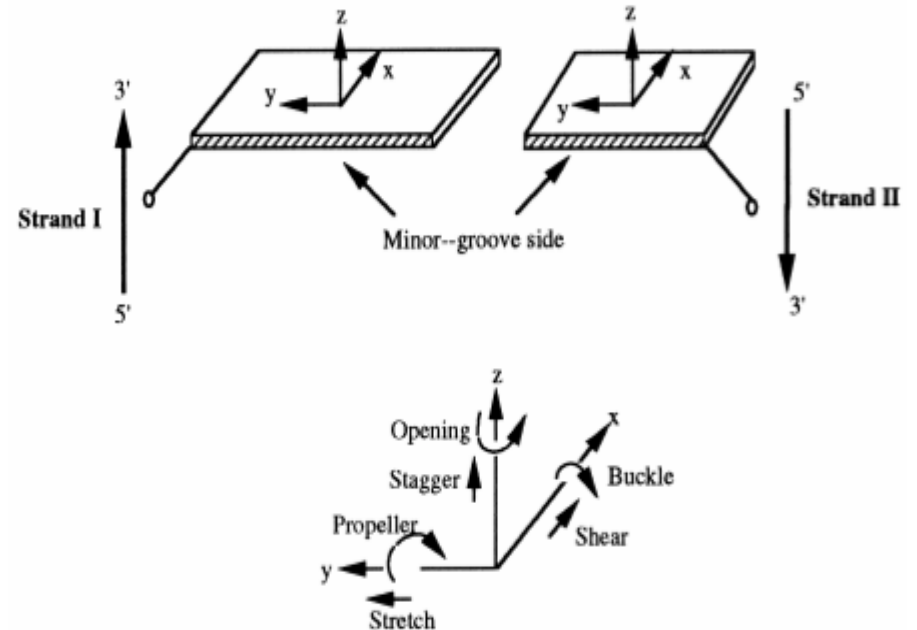
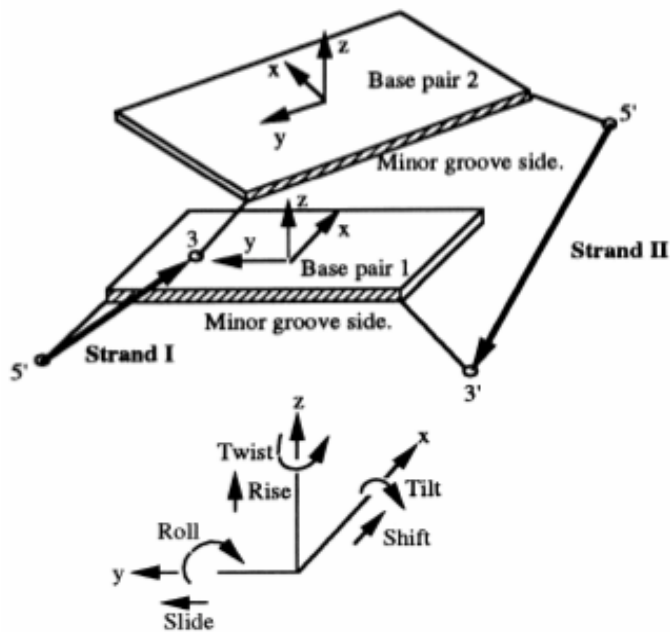
16 base-pairs



Chem. & Eng. News; July 17, 2006

ICM – Parameters

12 step parameters



ICM – How It Works

Configuration file

147 base-pairs

0 ***local base-pair & step parameters***

	Shear	Stretch	Stagger	Buckle	Prop	Opening	Shift	Slide	Rise	Tilt	Roll	Twist
T-A	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C-G	0.00	0.00	0.00	0.00	0.00	0.00	-0.07	-0.12	3.30	-0.47	5.91	33.56
T-A	0.00	0.00	0.00	0.00	0.00	0.00	-0.12	-0.04	3.30	-1.02	4.58	34.22

...

ICM – Calculations

Input into ICM

$$T_{i+1} = \left[R_z \left(\frac{\Omega}{2} - \phi \right) R_y(\Gamma) R_z \left(\frac{\Omega}{2} + \phi \right) \right] T_i$$

$$T_{mst} = \left[R_z \left(\frac{\Omega}{2} - \phi \right) R_y \left(\frac{\Gamma}{2} \right) R_z(\phi) \right] T_i$$

$$r_{i+1}^o = r_i^o + D_x x_{mst} + D_y y_{mst} + D_z z_{mst}$$

El Hassan & Calladine JMB 251 648-664 1995

ICM – Current

Limitations – Nucleosome choices

Revised ICM – Objectives

- More choices
- Move into different language
- Upload onto BitBucket to make it more accessible and to increase advertising for ICM

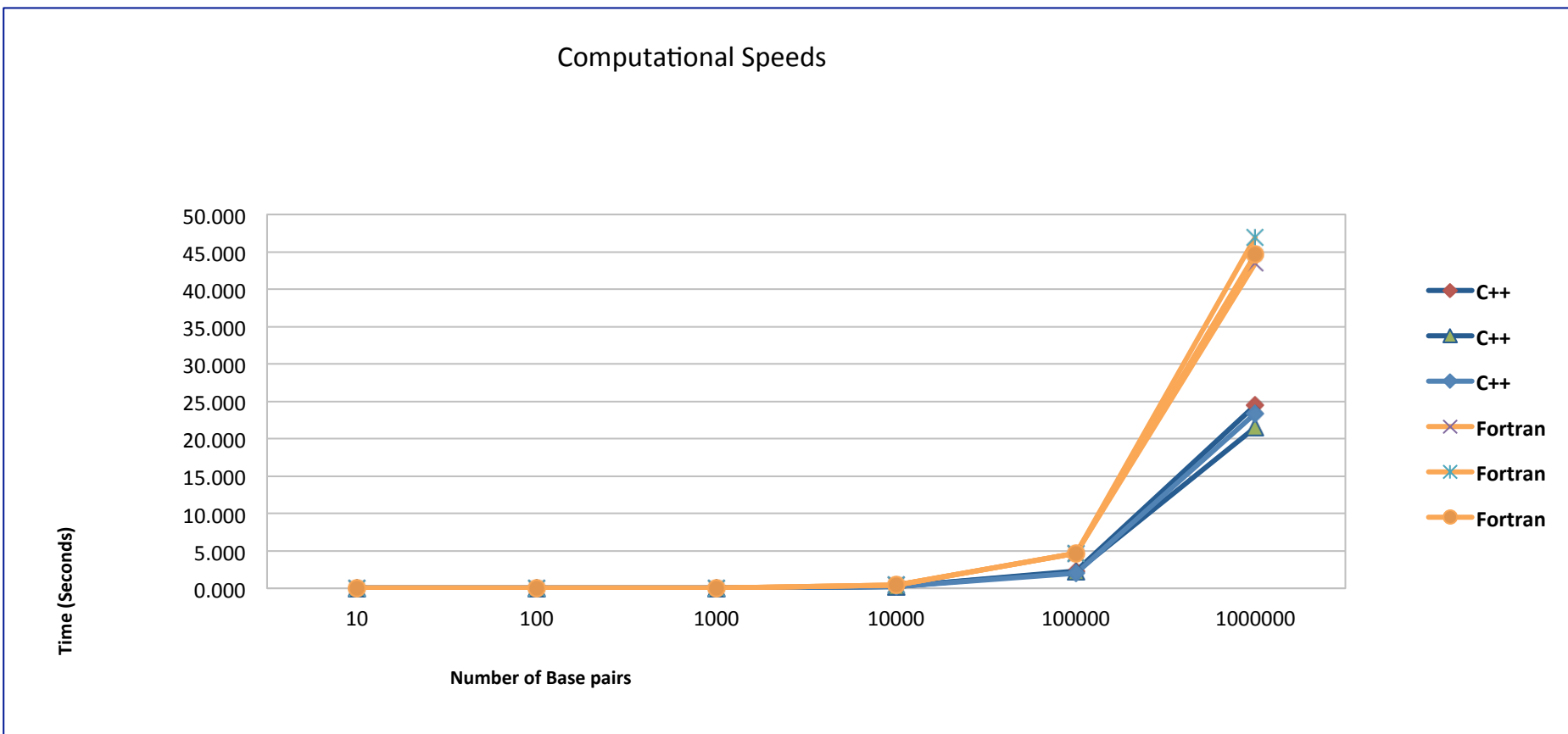
Revised ICM – More Visible

- Set up BitBucket
- Link to ICM Web and validate

Revised ICM – C++ vs FORTRAN

Experiment - Determine whether the program will run faster in C++.

ICM – C++ vs FORTRAN



# Base pairs		10	100	1000	10000	100000	1000000
C++	Test #1	0.000	0.003	0.017	0.205	2.005	23.382
	Test #2	0.001	0.003	0.022	0.205	2.301	24.485
	Test #3	0.000	0.003	0.017	0.197	2.226	21.498
Fortran	Test #1	0.000	0.006	0.047	0.467	4.646	43.507
	Test #2	0.000	0.006	0.044	0.457	4.662	46.937
	Test #3	0.001	0.009	0.049	0.472	4.682	44.637

ICM – C++ vs FORTRAN

Outcome – C++ faster

Relevance:

Genome		FORTRAN	C++	time
	1 million bp	45	25	sec
Yeast	12.1 million bp	9	5	mins
Human	3 billion bp	37.5	20.8	hours

ICM – Future Directions

Fully integrate C++

Modify ICM as knowledge increases

ICM – Acknowledgments

Mentor: Dr. Bishop

Co-workers: James Liman, William Johnston,
Victoria Bamburg, Rod Abcede

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