“The Scientific Computing Seminar is an interdisciplinary, student-oriented event which serves as a venue for dissemination of information about various aspects of scientific computing such as:

• applications of scientific computing to various disciplines, including some non-traditional ones,

• technical aspects of high-performance computing,

• tutorials concerning practical aspects of computing (hardware/software issues, code development, parallelization, debugging, etc.).

The selection of topics highlights both the breadth and depth of research in scientific computing at McMaster.”
COMPUTATIONAL BIOLOGY

- identify problem
- conceptualise approach
- encode ideas
- validate with data
- conduct simulations
- admit limitations
- refine iteratively
THE FIRST ECHINOID

By HERBERT L. HAWKINS, D.Sc., F.G.S.

Professor of Geology in the University of Reading.

(Received April 7, 1931.)

(With Two Text-figures.)
sea urchin skeleton (test)

- interambulacral column
- apical system
- plates
- ambulacral column
body symmetry among animals

(a) Asymmetry

Sponge

No plane of symmetry
(b) Radial symmetry

Jellyfish

Multiple planes of symmetry
(c) Bilateral symmetry

Lizard

Single plane of symmetry

Posterior

Anterior
animal evolutionary diagram (phylum level) – DNA sequence data

Phylogenetic tree based on similarities and differences in the DNA sequences of several genes from various animal phyla. The bars along the branches indicate when certain morphological traits originated.
Phylogenetic tree based on similarities and differences in the DNA sequences of several genes from various animal phyla. The bars along the branches indicate when certain morphological traits originated.
“I hereby salute the echinoderm as a noble group especially designed to puzzle the zoologist.”
echinoid evo-devo
COMPUTATIONAL BIOLOGY

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1. gapping
2. addition
3. accretion
4. interaction
5. visceral growth

"D'Arcy Thompson surely stands as the most influential biologist ever left on the fringes of legitimate science."
1. gapping
2. addition
3. accretion
4. interaction
5. visceral growth
bubble analogy
plate gapping
close packing
circle packing

tesselation: triangle or square
Descartes’ theorem

\[ d = \frac{abc (bc + a(b + c) - 2\sqrt{a}\sqrt{b}\sqrt{c}\sqrt{a+b+c})}{a^2 (b-c)^2 + b^2 c^2 - 2abc(b+c)} \]
Fermat point
\[ |PA| + |PB| + |PC| = \text{minimum} \]
Fermat point

Descartes’ theorem

= circle packing
plate addition
$P = \frac{a}{1 + e^{(c(b-T))}}$
plate accretion
Distance from Apical System

Growth increments

Distance vs. Growth Increments
plate interaction
Young-Laplace equation

\[ p = \frac{2\sigma}{r} \]
equal size

unequal size
\[ \frac{1}{r_B} = \frac{1}{r_A} + \frac{1}{r_C} \]
cosine law
COMPUTATIONAL BIOLOGY

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2D projection
geometric representation
plate gapping
plate addition

Figure captions:

a, c: Images showing different stages of plate addition.
b, d: Diagrams illustrating the process of plate addition with labels for ap, ge, oc, inp, and anp.
plate accretion
plate interaction
Ambulacral Plate Number

4

6

10
COMPUTATIONAL BIOLOGY

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• conduct simulations
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ambitus position
COMPUTATIONAL BIOLOGY

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computer simulation

tpn = 40; \( \alpha_{gz} = 72^\circ \); \( ap_r = 0.05 \text{ mm} \); \( ps:ap_r = 1 \); \( ap_r:cl = 0 \)

\( \alpha_{am} = 20^\circ \)

\( \alpha_{am} = 31^\circ \)
computer simulation – growth zones

tpn = 40; \( \alpha_{gz} = 72^\circ \); \( ap_r = 0.05 \text{ mm} \)

\( \alpha_{am} = 16^\circ \)
\( ps : ap_r = 1.33 \)
\( ap_r : cl = 0.18 \)

\( \alpha_{am} = 20^\circ \)
\( ps : ap_r = 1.97 \)
\( ap_r : cl = 0.14 \)

\( \alpha_{am} = 32^\circ \)
\( ps : ap_r = 2.5 \)
\( ap_r : cl = 0.09 \)

\( \alpha_{am} = 39^\circ \)
\( ps : ap_r = 0.53 \)
\( ap_r : cl = 0.04 \)
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LIMITATIONS

• plates analogised and represented as bubbles
• plates added with prescribed numbers, locations, rates
• single growth zone considered
• biserial column morphologies
• ambulacral plates represented as three circles
• two-dimensional projection (for 3D penta-growth-zones)
• prescribes ratios $ps:ap_r$, $ap_r:cl$
COMPUTATIONAL BIOLOGY

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