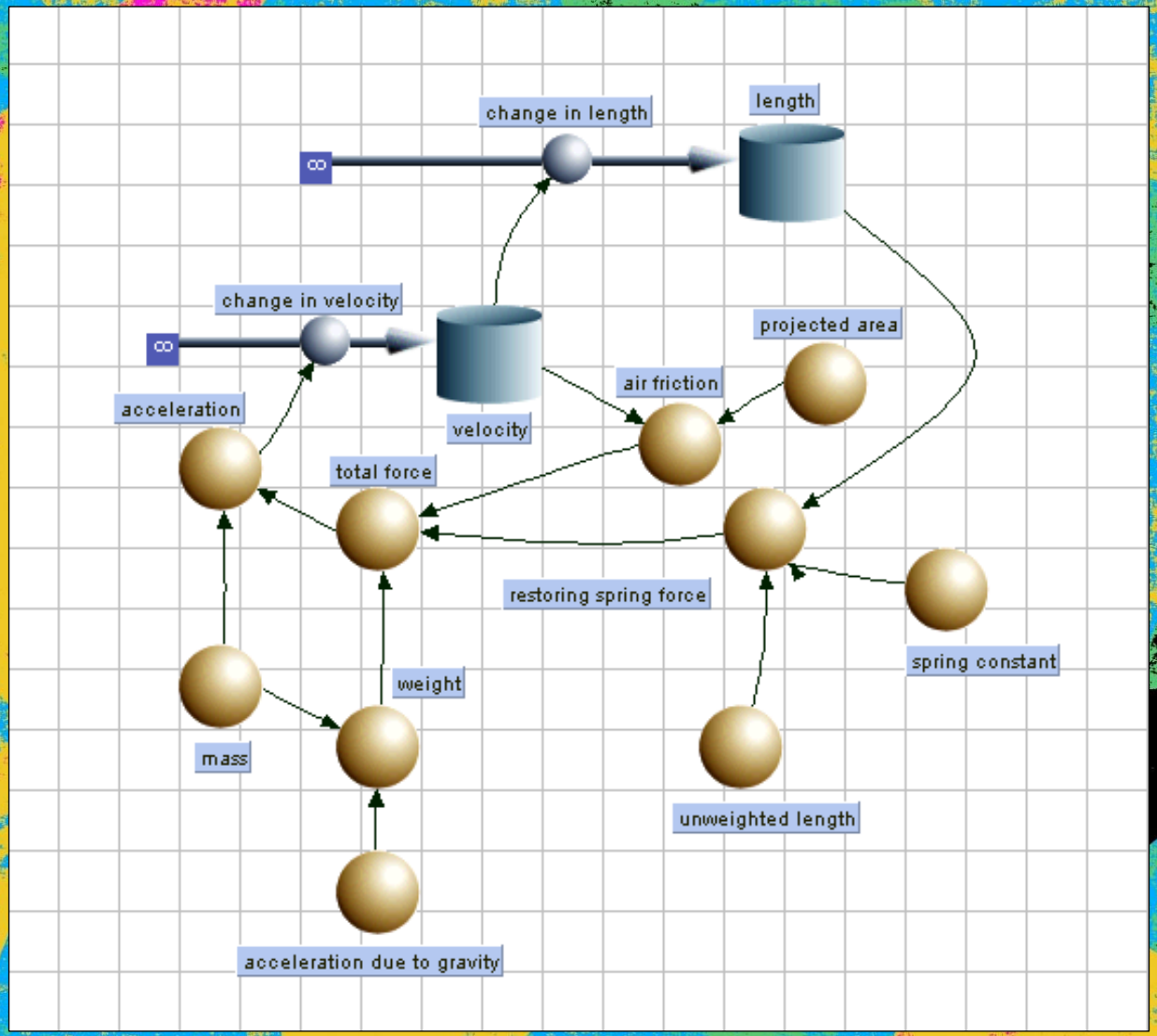
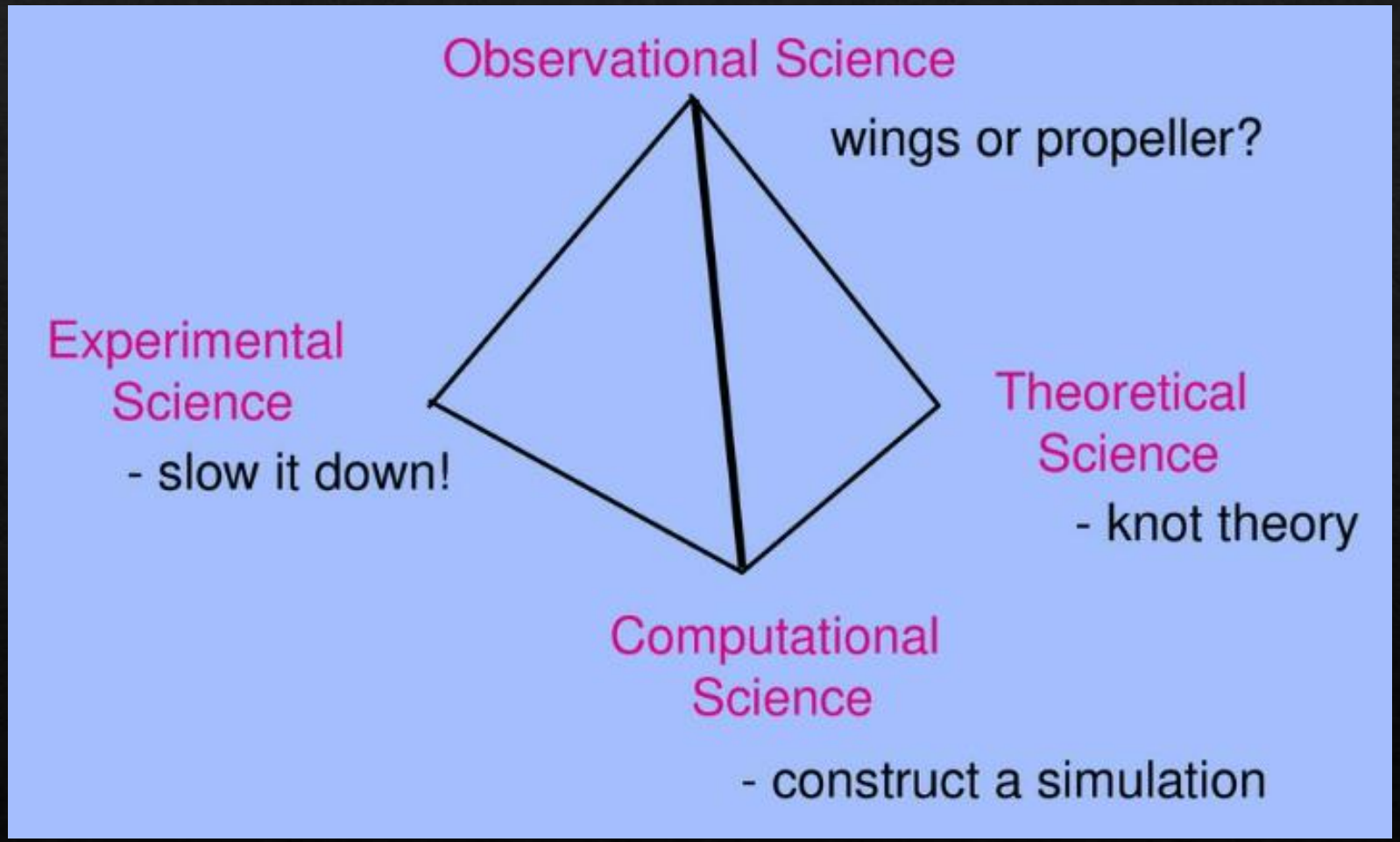
Introduction to Computational Science

CS 313 Computational Science

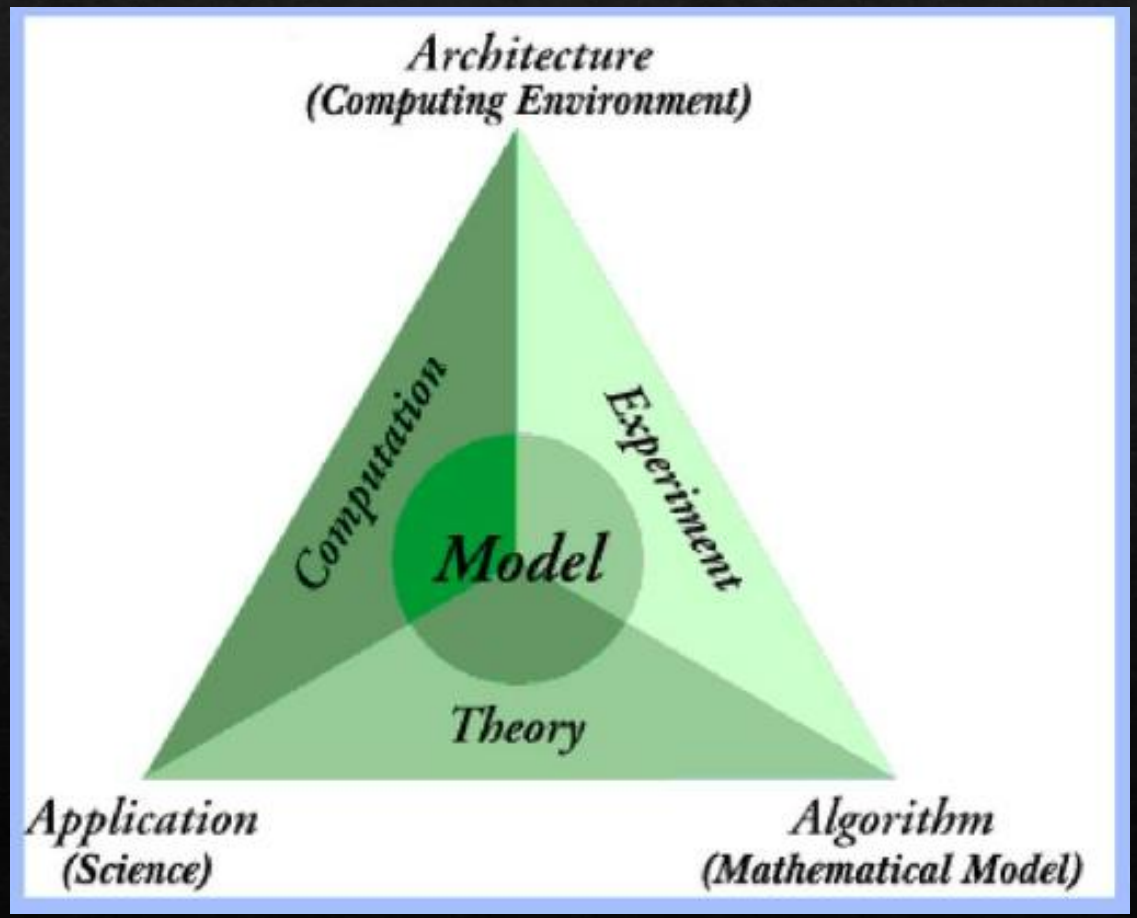
1st Sem. A.Y. 2022 - 2023



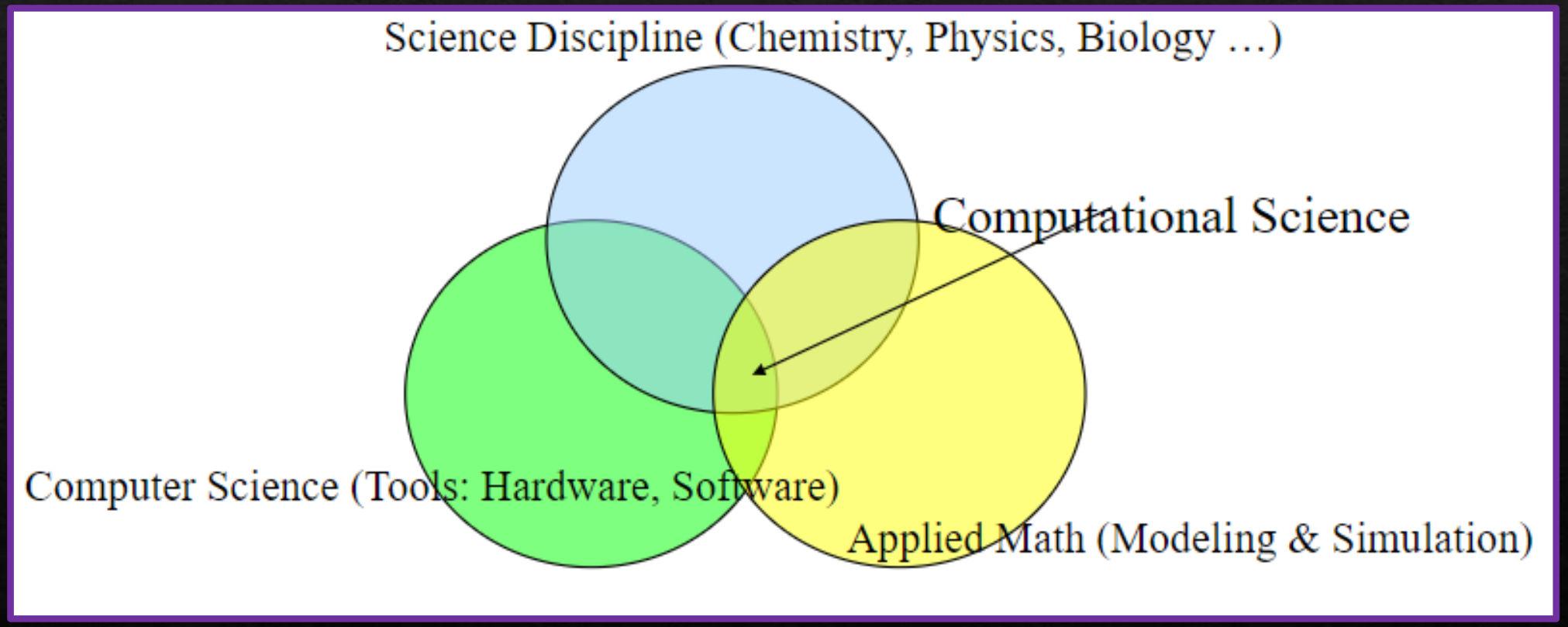
SCIENCE : the study of how nature behaves



Computational Science : A Tripartite Approach

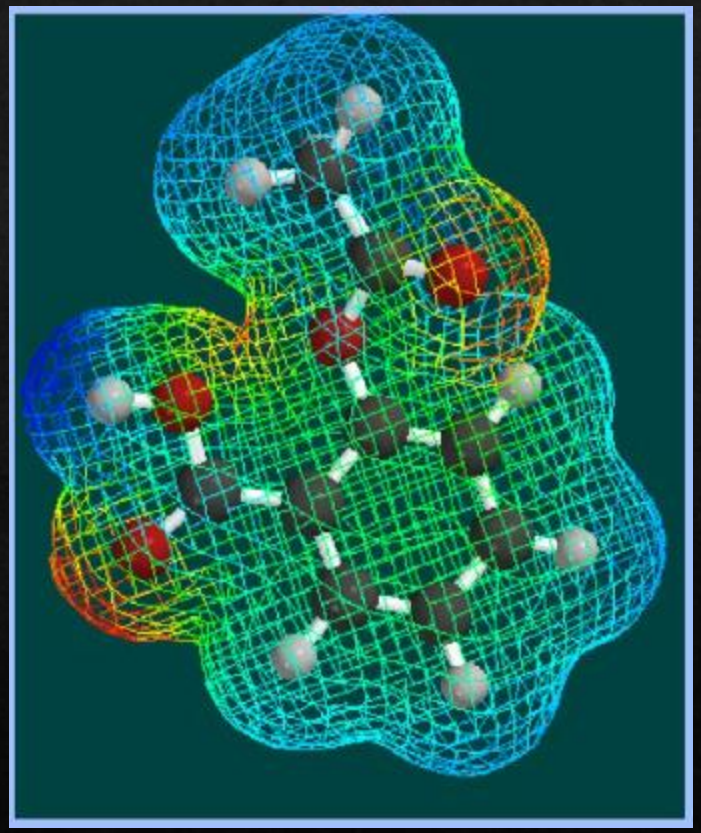


Computational Science : A Tripartite Approach



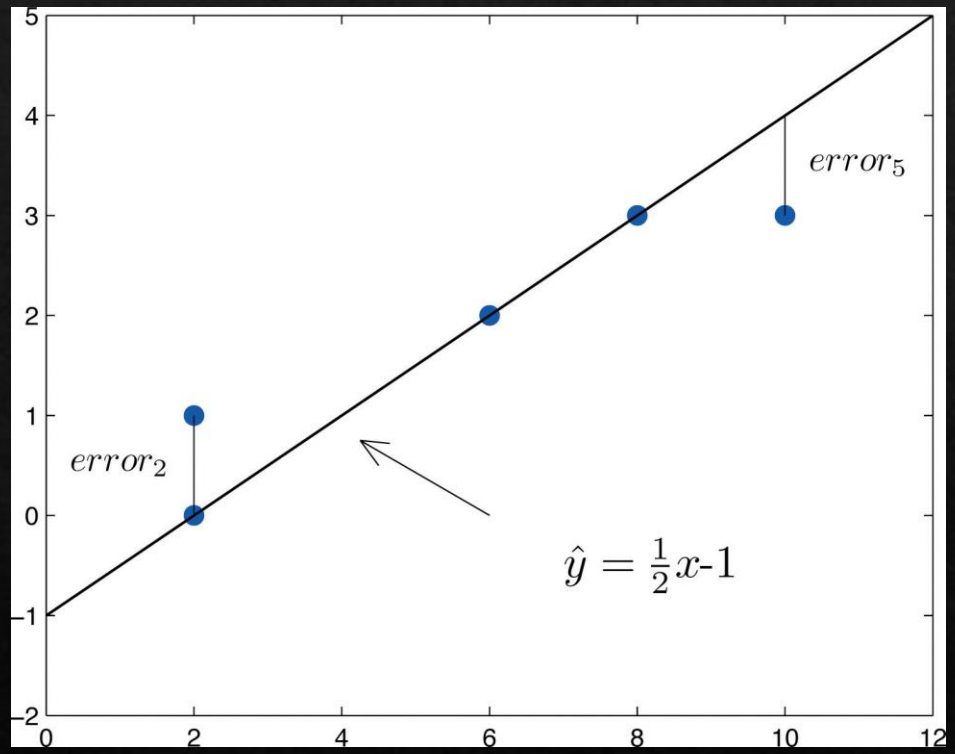
Applications

- Chemistry: electronic structure determinations
- Physics: astrophysics (galaxy simulations)
- Biology: population dynamics
- Environmental Science: acid rain deposition models
- Political Science/History: causative factors in Bosnian War conflict
- Medicine: epidemiology, pharamacokinetics models



Algorithms

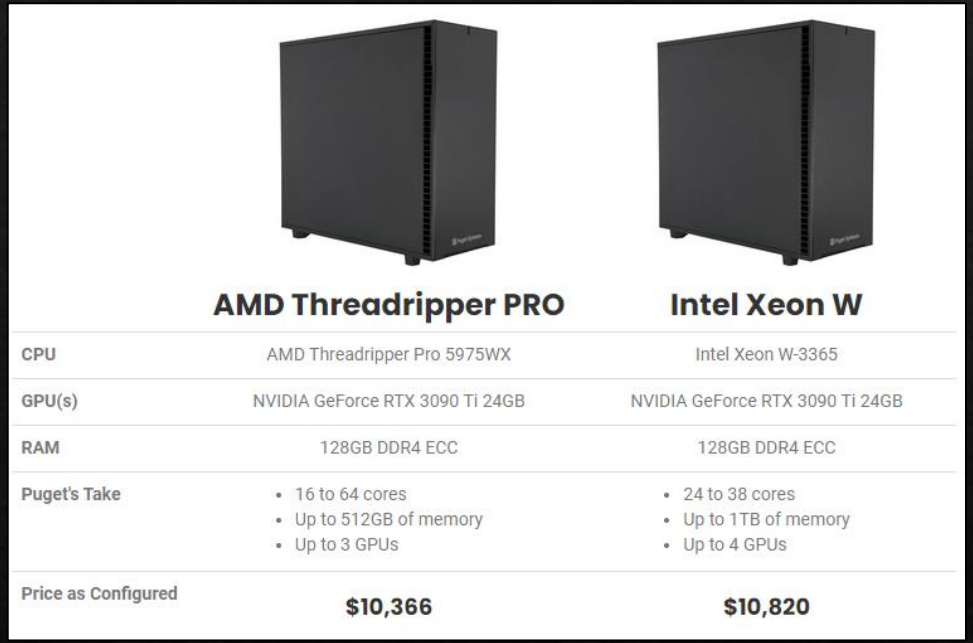
- Creating a mathematical representation of the problem – the "mathematical model"
- Choosing the appropriate numerical "recipe" to solve the problem
  - Linear Least Squares: for fitting data to a line
  - Newton's Method: for finding roots of an equation
  - Euler's Method: for solving integrals
  - Cramer's Rule: for solving systems of equations



The Least Squares Regression Line

Architecture

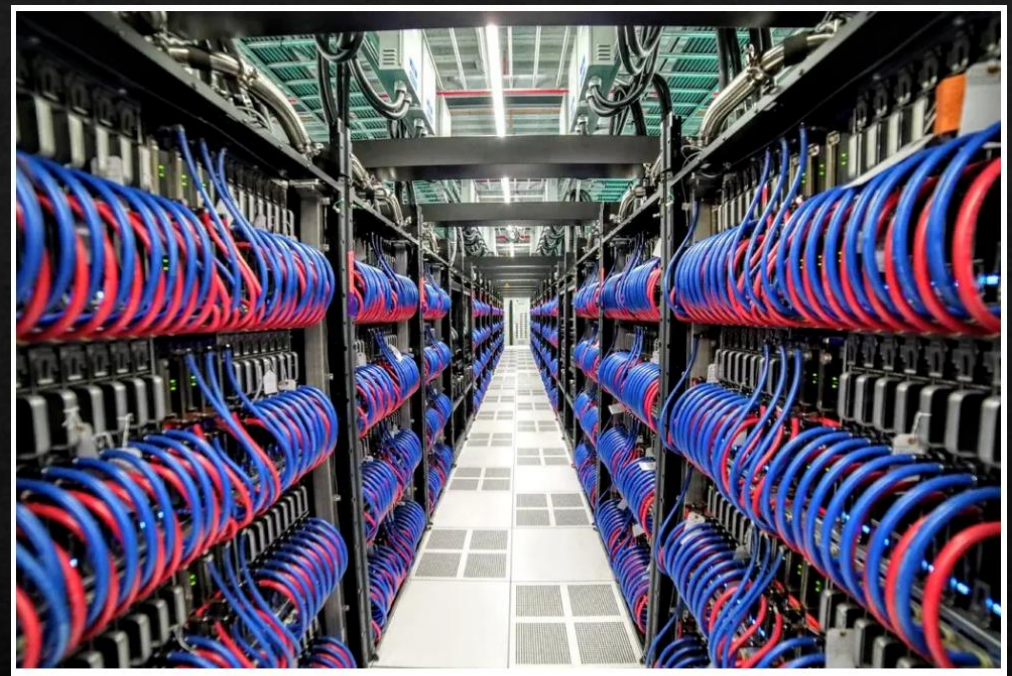
- Choosing the appropriate "platform" to solve the problem
  - Single-user personal computer : (Macbook Pro, Dell, Lenovo, etc.)
  - Scientific workstation: (ex. Puget Systems)
  - Supercomputer: for solving integrals
  - High Performance Computing (HPC): for solving systems of equations



	AMD Threadripper PRO	Intel Xeon W
CPU	AMD Threadripper Pro 5975WX	Intel Xeon W-3365
GPU(s)	NVIDIA GeForce RTX 3090 Ti 24GB	NVIDIA GeForce RTX 3090 Ti 24GB
RAM	128GB DDR4 ECC	128GB DDR4 ECC
Puget's Take	• 16 to 64 cores • Up to 512GB of memory • Up to 3 GPUs	• 24 to 38 cores • Up to 1TB of memory • Up to 4 GPUs
Price as Configured	**$10,366**	**$10,820**

Architecture

- Choosing the appropriate "platform" to solve the problem
  - Single-user personal computer : (Macbook Pro, Dell, Lenovo, etc.)
  - Scientific workstation: (ex. Puget Systems)
  - Supercomputer: (ex. Frontier)
  - High Performance Computing (HPC): hundreds or thousands of computer servers are networked together.



Frontier, the world's largest supercomputer, relies on a cooling system that uses 6,000 gallons of water a minute. Image: Oak Ridge National Laboratory/Hewlett Packard Enterprise

Simple Example: Tying your shoe

- Application: what is the science of tying a shoe?
- Architecture: a computational schoe
- Algorithm: determining the mathematics
  - Variables?
  - Assumptions?

$$TYS = \frac{A}{B} + \frac{0.5A}{0.5B}$$

A Computational Geode!

- Application: the “jewel”
- Architecture: the “tool”
- Algorithm: the “rule”

More about geodes: https://sciencing.com/geodes-5377367.html

Computational Science Tools

- Type of tools for solving computational problems
  - Programming: Python, R, FORTRAN, C/C++, Matlab
  - Equation-Solvers: Matlab, Mathematica, Octave, Maple, MathCAD
  - Dynamic Modelers: Berkeley Madonna, Stella, Vensim
  - Scientific Visualization Programs: Matlab, FAST, XMol

    More here: http://www.cs.cmu.edu/~yanxi/vis.html
  - Discipline-Specific Software: ANALYZE, AIPS, VIS-5D

A Sample Problem: Behavior of Gases (Chemistry)

- Ideal Gas Law: PV = nRT
  - pressure * volume = amount of gas * constant * temperature
- This mathematical model makes two assumptions about gases
  - gas molecules in a closed container will never bump into each other
  - we can compress the molecules down to a volume of zero
- Need a better mathematical model for understanding the behavior of gases
  - van der Waals
  - Beattie-Bridgeman
  - Redlich-Kwong

Van der Waals equation

- Takes into account the two assumptions by adding two new constants, *a* and *b*
- Generates a mathematical equation that is very difficult to solve analytically (using algebra)
- Van der Waals equation: $\left(P + a\frac{n^2}{V^2}\right)(V - nb) = nRT$
- The problem is to choose a way to solve this computationally
  - we know the application we wish to solve
  - We know the algorithms (we have the mathematical model)
  - we need to select the architecture and the tool
    - ✓ Architecture: PCs are powerful enough!
    - ✓ A variety of tools can be used!

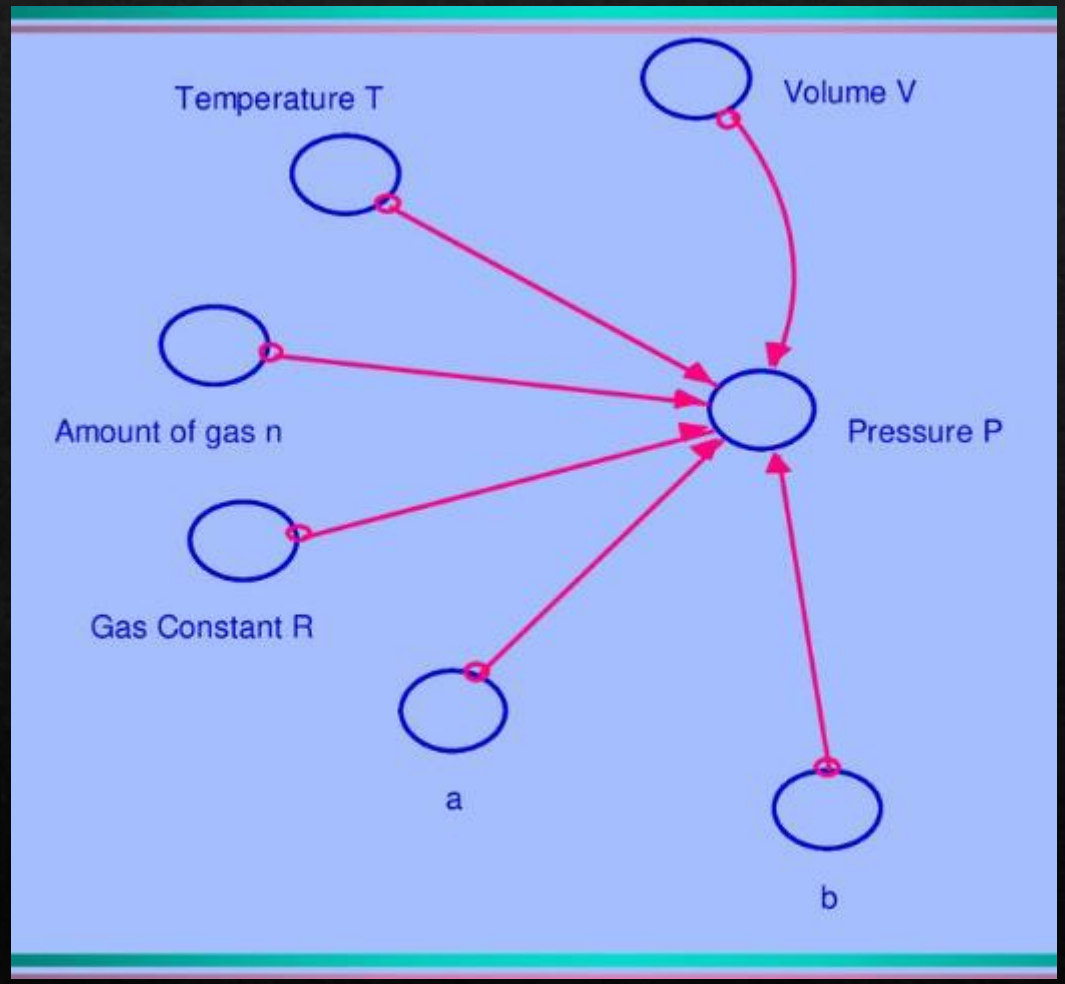
Spreadsheet Implementation

	A	B	C
1	GAS LAWS EQUATIONS OF STATE		
2			
3	n =	1	
4	R =	0.0820575	
5	T =	302.15	
6			
7	a =	3.592	
8	b =	0.04267	
9			
10	Vo =	1	
11	dV =	1	
12			
13		Ideal	van der Waals
14		Gas Law	Equation
15	Volume	Pressure	Pressure
16	1	24.793674	
17	2	12.396837	11.76909
18	3	8.264558	7.98469
19	4	6.198418	6.04075
20	5	4.958735	4.85774
21	6	4.132279	4.06210
22	7	3.541953	3.49037
23	8	3.099209	3.05970
24	9	2.754853	2.72363
25	10	2.479367	2.45407
26			

Fortran Implementation

```
      PROGRAM NEWTON
C
C     ***************************************************************
C     THIS PROGRAM ILLUSTRATES THE NEWTONS METHOD FOR SOLVING THE
C     VAN DER WAALS EQUATION OF STATE.  COIFFICIENTS A0, A[1..3] ARE
C     DETERMINED FROM INPUT VALUES A,B,T, AND P<=PP<=PFINAL AS WELL
C     AS PARAMETER R
C     ***************************************************************
      IMPLICIT NONE
      DOUBLE PRECISION
A,B,V0,V,P,PINC,PFINAL,PP,T,RT,AB,R,EPS,COEF0,COEF(3)
      LOGICAL ERROR
      PARAMETER (R=8.0205D-2,EPS=1.0D-5)
      READ *,A,B,T,P,PINC,PFINAL
      AB=A*B
      RT=R*T
      DO 3 PP=P,PFINAL,PINC
        V0=RT/PP
        COEF(3)=1
        COEF(2)=-1*(B+RT/PP)
        COEF(1)=A/PP
        COEF0=-1*AB/PP
        CALL NEIT(V0,V,COEF,COEF0,EPS,ERROR)
        IF (.NOT. ERROR) PRINT *,PP,V
        CALL NEIT(0,V,COEF,COEF0,EPS,ERROR)
        IF (.NOT. ERROR) PRINT *,PP,V
3     CONTINUE
      STOP
      END
C     ***************************************************************
      SUBROUTINE NEIT(V0,V,COEF,COEF0,EPS,ERROR)
      DOUBLE PRECISION V0,V,COEF(3),COEF0,EPS,F,DF
      INTEGER ITS
      LOGICAL ERROR
```

Stella Implementation



MathCAD Implementation

GAS LAWS EQUATIONS OF STATE:

This model looks at the relationship: PV=nRT, where P is the pressure of the gas, V is the volume of the gas, n is the amount of gas, R is a gas constant, and T is the temperature.

$n := 1$

$R := 0.0820575$

$T := 302.15$

$a := 3.592$

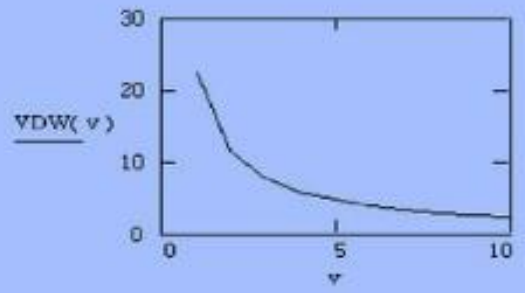
$b := 0.04267$

$v := 1, 2 .. 10$

$idgl(v) := \frac{n \cdot R \cdot T}{v}$

$VDW(v) := \frac{n \cdot R \cdot T}{(v - (n \cdot b))} - \frac{n^2 \cdot a}{v^2}$

idgl(v)	VDW(v)
24.794	22.307
12.397	11.769
8.265	7.985
6.198	6.041
4.959	4.858
4.132	4.062
3.542	3.49
3.099	3.06
2.755	2.724
2.479	2.454



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What Computational Science is NOT!

- Putting numbers into spreadsheet
- Analyzing data gathered in the field or experimentally
- Fitting data to an equation
- Visualizing data collected experimentally or in the field
- Writing a computer program
- Using a computer to do databases, word processing or presentations

Why do we need this?

- There are many interesting problems that can be solved using this technology that cannot be easily solved using traditional methods
  - Too tedious to solve problems using calculators
  - Too dangerous to try to solve problems in the laboratory
  - Too expensive to try to solve in the laboratory
  - Problems are only solvable using mathematical techniques or tools
- Establish a true marriage between mathematics, computing and science.
- Who cares?

Who cares?

- 21st Century Science: The Grand Challenges
  - Molecular and structural biology
  - Cosmology
  - Environmental Hydrology
  - Warfare and Survivability
  - Chemical Engineering and chemical structure
  - Weather prediction
  - Nanomaterials
- Solve any PART of these problems, and …

You might win THIS