CM3110
Transport Processes and Unit Operations I

Numerical methods in transport phenomena/chemical engineering

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Department of Chemical Engineering
Michigan Technological University

www.chem.mtu.edu/~fmorriso/cm310/cm310.html

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Numerical methods in transport phenomena/chemical engineering

- Numerical integration (one-dimensional; trapezoidal rule)
- Optimization (Excel Solver)
- Iterative Problem Solving
- Numerical integration (two-dimensional; finite-element package Comsol)

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Numerical methods in transport phenomena/chemical engineering

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•Numerical integration (one-dimensional; trapezoidal rule)

•Optimization (Excel Solver)

•Iterative Problem Solving

•Numerical integration (two-dimensional; finite-element package Comsol)

(easy on a calculator, but sometimes it is part of a larger calculation . . . . .)

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An example from Rheology (Binding Analysis)

Calculate the following integral for known *n* and *t*

$$I_{nt} = \int_0^1 \left| 2 - \left(\frac{3n+1}{n} \right) \varphi^{1+1/n} \right|^{t+1} \varphi \, d\varphi$$

$$I_{nt} = \int_a^b f(\varphi) d\varphi$$

Use trapezoidal rule.

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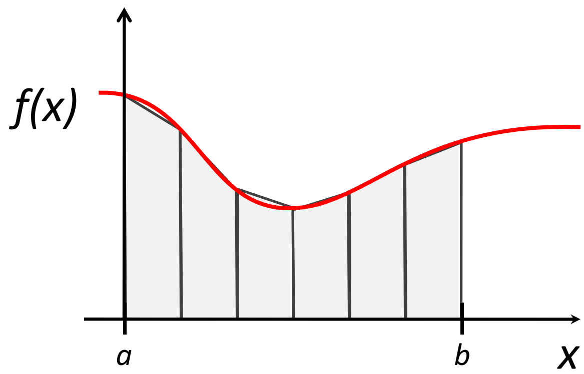
Trapezoidal Rule

$$I = \int_a^b f(x)\,dx$$



$$\frac{dy}{dx} = f(x)$$

$$y(x) = I = Area = \sum \tfrac{1}{2}(b_1 + b_2)h$$

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$$I_{nt} = \int_0^1 \left| 2 - \left(\frac{3n+1}{n}\right)\varphi^{1+1/n} \right|^{t+1} \varphi\, d\varphi$$

$$area = \tfrac{1}{2}(b_1 + b_2)h$$

Trapezoidal rule integration

PL_n=	0.48
PL_m=	6,982.50
T_guess=	1.25
Ratio3=(3*n+1)/n=	5.07
Integral=	1.36

Integral=sum of areas column

$\Delta\phi$=	0.005	
phi	**f(phi)**	**areas**
0	0.0000000	
0.005000	0.0237465	0.000059
0.010000	0.0474928	0.000178
0.015000	0.0712385	0.000297
0.020000	0.0949827	0.000416
0.025000	0.1187244	0.000534
0.030000	0.1424618	0.000653
0.035000	0.1661933	0.000772
0.040000	0.1899165	0.000890
0.045000	0.2136289	0.001009
0.050000	0.2373273	0.001127
0.055000	0.2610086	0.001246
0.060000	0.2846689	0.001364
0.065000	0.3083041	0.001482
0.070000	0.3319097	0.001601
0.075000	0.3554809	0.001718
0.080000	0.3790123	0.001836
0.085000	0.4024983	0.001954
0.090000	0.4259328	0.002071
0.095000	0.4493095	0.002188
0.100000	0.4726216	0.002305
0.105000	0.4958618	0.002421

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- **Optimization (Excel Solver)**
- Iterative Problem Solving
- Numerical integration (two-dimensional; finite-element package Comsol)

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Detailed handout is on the web

http://www.chem.mtu.edu/~fmorriso/cm4650/Using_Solver_in_Excel.pdf

Using the *Solver* Add-in in Microsoft Excel®

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February 15, 1999
Modified April 12, 2005

If you have a nonlinear model with adjustable parameters and some data you would like to fit the model to, the *Excel®* *Solver* option is a very nice way to carry out the fit. I would like to thank Michael Hickner MTU '99 for showing me how to do this and Charles Lusignan from Eastman Kodak for some helpful insights.

As an example, consider the Carreau-Yasuda model for viscosity of a non-Newtonian fluid:

$$\eta(\dot{\gamma}) = \eta_\infty + (\eta_o - \eta_\infty)\left[1 + (\dot{\gamma}\lambda)^a\right]^{\frac{n-1}{a}}$$

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Basic idea: minimize the error between the values predicted by a model and the data that you have.

$$\text{Value to be minimized by Solver} = \sum_{\text{all data}} \frac{(\text{model} - \text{data})^2}{(\text{data})^2}$$

The minimization is achieved by manipulating parameters of the model.

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Optimization with Excel Solver

1. Office button
2. Excel Options
3. Add-ins, Excel add-ins, Go. (Solver installed; do once only)
4. Set up error cell (*Target Cell*)
5. Select: *Data*, *Solver*
6. Choose parameters that Solver manipulates (optimizes) to minimize the *Target Cell*)
7. Select: *Options*, *Use Automatic Scal*ing
8. Solve

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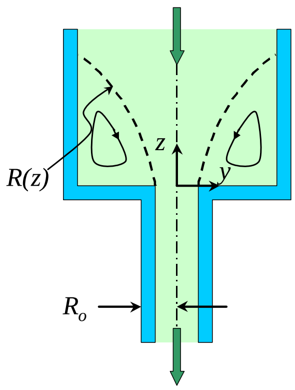
Binding Analysis (rheology)



From measurements of entrance pressure loss versus flow rate, estimate the two parameters *t* and *l* in the elongational viscosity model. The two parameters *n* and *m* from the shear viscosity model are known.

shear stress $\tau_R = m\dot{\gamma}_a^n$

elongation viscosity $\bar{\eta} = l\dot{\varepsilon}_o^{\,t-1}$

D. M. Binding, JNNFM (1988) 27, 173-189.

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Binding Analysis (rheology)

$$\eta = l\dot{\varepsilon}_o^{t-1}$$

$$\eta = m\dot{\gamma}_a^{n-1} \qquad \alpha = \frac{R_0(capillary)}{R_1(barrel)}$$

$$\Delta p_{ent} = \frac{2m(1+t)^2}{3t^2(1+n)^2}\left\{\frac{lt(3n+1)n^t I_{nt}}{m}\right\}^{1/(1+t)} \dot{\gamma}_{R_o}^{\;t(n+1)/(1+t)}\left\{1-\alpha^{3t(n+1)/(1+t)}\right\}$$

$$\dot{\gamma}_{R_o} = \frac{(3n+1)\,Q}{n\pi R_o^3}$$

$$I_{nt} = \int_0^1 \left|2-\left(\frac{3n+1}{n}\right)\phi^{1+1/n}\right|^{t+1} \phi\, d\phi$$

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Binding Analysis

Evaluation Procedure

1. Shear power-law parameter n must be known; must have data for Δp_{ent} versus Q
2. Guess t, l
3. Evaluate I_{nt} by numerical integration over f
4. Using Solver, find the best values of t and l that are consistent with the Δp_{ent} versus Q data

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Binding Analysis (rheology)

Known: $\alpha = \frac{R_0}{R_1}, n, m$

Data for $\Delta p_{ent}(Q)$

$$Ratio1 \equiv \frac{2m(1+t)^2}{3t^2(1+n)^2}$$

$$Ratio2 \equiv \frac{lt(3n+1)n^t}{m}$$

$$myExp1 \equiv t(n+1)/(1+t)$$

$$myExp2 \equiv 1/(1+t)$$

What are the best values of t and l so that the model is consistent with the $\Delta p_{ent}(Q)$ data?

$$\dot{\gamma}_{R_o} = \left(\frac{(3n+1)}{n\pi R_o^3}\right)Q$$

$$\Delta p_{ent} = (Ratio1)\left\{(Ratio2)I_{nt}\right\}^{myExp2} \dot{\gamma}_{R_o}^{\ myExp1}\left\{1-\alpha^{3\cdot myExp1}\right\}$$

Need to repeatedly evaluate the integral as we optimize the values of t and l.

$$I_{nt} \equiv \int_0^1 \left|2-\left(\frac{3n+1}{n}\right)\varphi^{1+1/n}\right|^{t+1} \varphi\, d\varphi$$

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Binding Analysis – using Excel Solver

Evaluate integral numerically

$$I_{nt} = \int_0^1 \left| 2 - \left(\frac{3n+1}{n} \right) \phi^{1+1/n} \right|^{t+1} \phi \, d\phi$$

phi	f(phi)	areas
0	0	
0.005	0.023746502	5.93663E-05
0.01	0.047492829	0.000178098
0.015	0.071238512	0.000296828
0.02	0.094982739	0.000415553
0.025	0.118724352	0.000534268
0.03	0.142461832	0.000652965
0.035	0.166193303	0.000771638
0.04	0.189916517	0.000890275
0.045	0.213628861	0.001008863
0.05	0.237327345	0.001127391
0.055	0.261008606	0.00124584
0.06	0.2846689	0.001364194
0.065	0.308304107	0.001482433

. . .

$$area = \frac{1}{2}(b_1 + b_2)h$$

Summing:

Int=	1.36055

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Binding Analysis – using Excel Solver

Optimize *t*, *I* using Solver

By varying these cells:

$$\frac{(predicted - actual)^2}{(actual)^2}$$

t_guess=	1.2477157	
I_guess=	11991.60895	
******* SOLVER SOLUTION ********		
predicted DeltaPent	exptal DeltaPent	difference
1.26E+06	1.13E+06	1.35E-02
6.88E+05	7.43E+05	5.51E-03
5.43E+05	5.88E+05	6.02E-03
3.89E+05	4.55E+05	2.14E-02
2.78E+05	2.54E+05	9.28E-03
	target cell	5.57E-02

Sum of the differences: Minimize this cell

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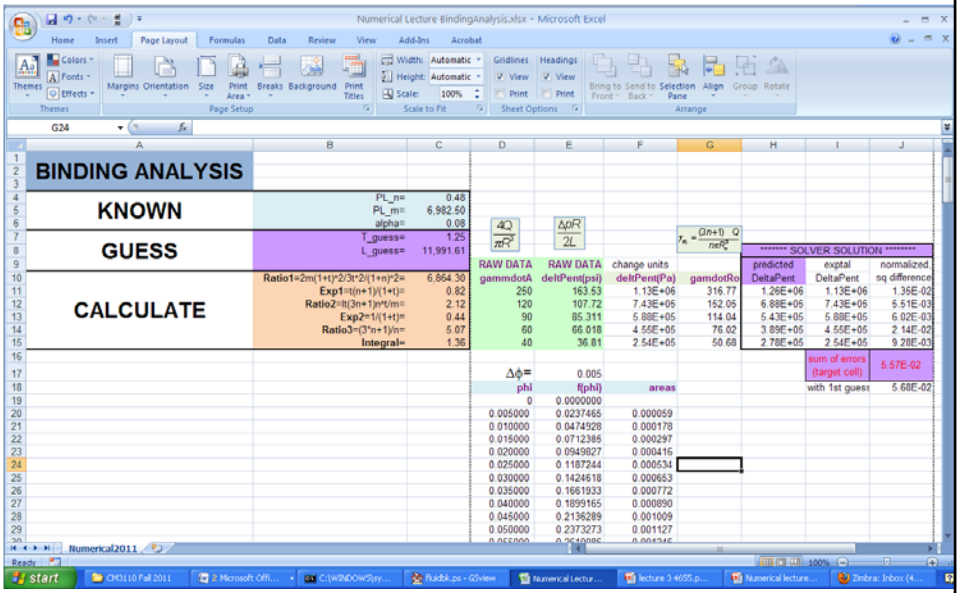

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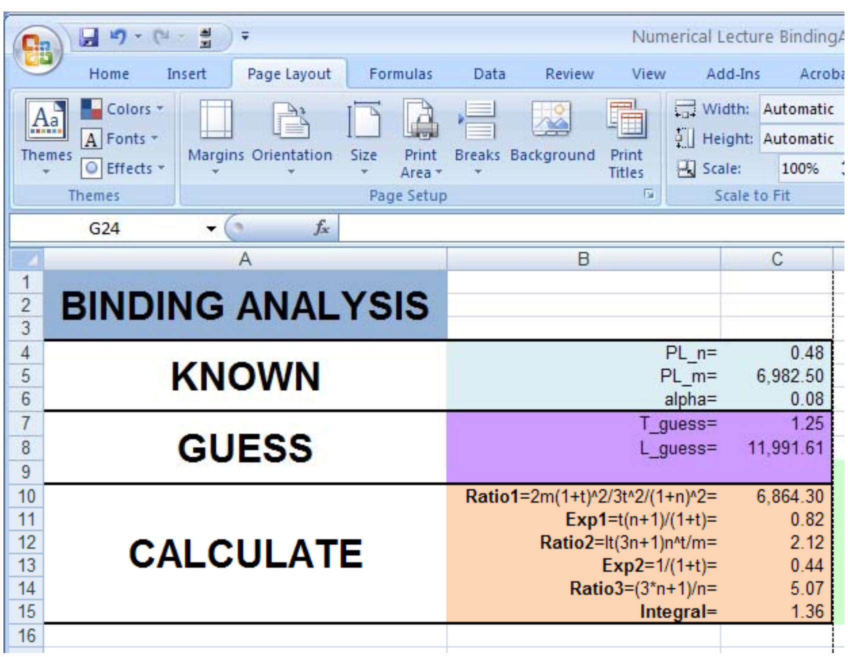

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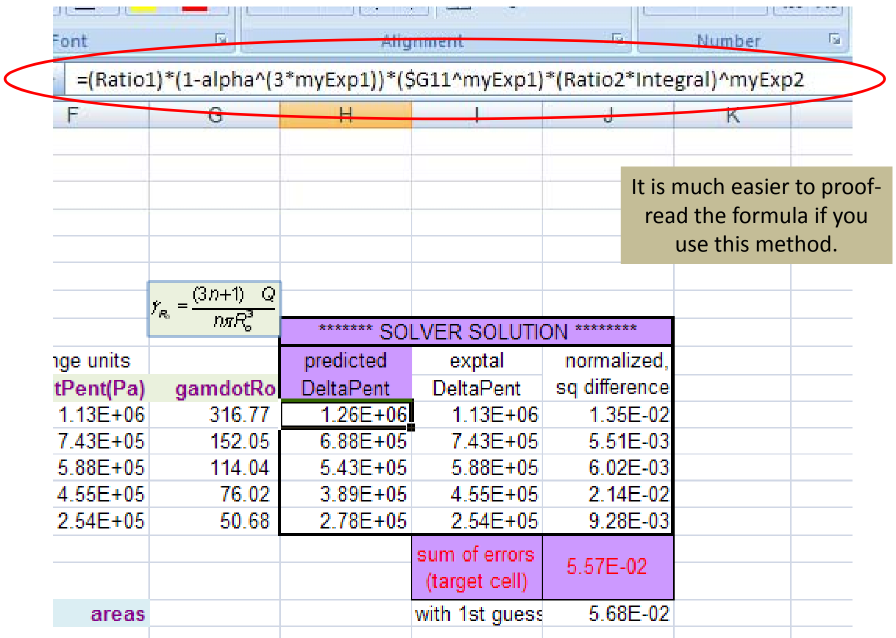

... ge units		predicted	exptal	normalized,
tPent(Pa)	gamdotRo	DeltaPent	DeltaPent	sq difference
1.13E+06	316.77	1.26E+06	1.13E+06	1.35E-02
7.43E+05	152.05	6.88E+05	7.43E+05	5.51E-03
5.88E+05	114.04	5.43E+05	5.88E+05	6.02E-03
4.55E+05	76.02	3.89E+05	4.55E+05	2.14E-02
2.54E+05	50.68	2.78E+05	2.54E+05	9.28E-03
			sum of errors (target cell)	5.57E-02
areas			with 1st guess	5.68E-02

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Good Excel Habits:

- Break formulas into chunks that are easier to check
- Name cells so that the names appear in the formulas (easier to check)
- Do unit conversions explicitly rather than hidden in formulas

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Iterative Problem Solving with Excel 2007

1. Office button 
2. Excel Options
3. Formulas
4. Calculation Options
5. Select: *Manual recalculation*
6. Select: *Enable Iterative Calculation*; *Maximum iterations = 1*
7. Set a circular reference
8. Use *F9* to recalculate one step at a time

WARNING: Don't forget you are in Manual recalculation mode

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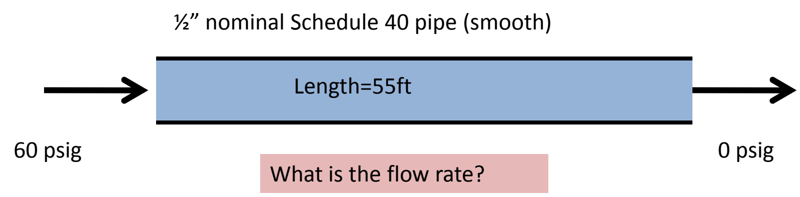
Example: Calculate flow rate in a pipe from a known pressure drop



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Data correlation for friction factor (ΔP) versus Re (flow rate) in a pipe

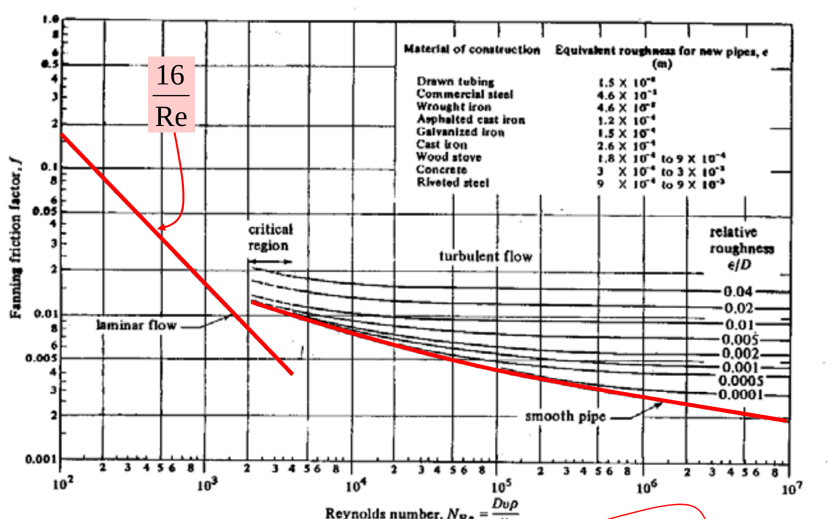

FIGURE 2.10-3. *Friction factors for fluids inside pipes. [Based on L. F. Moody, Trans. A.S.M.E., 66, 671, (1944); Mech. Eng. 69, 1005 (1947). With permission.]*

(Geankoplis, 1993, p88)

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Data are organized in terms of two dimensionless parameters:

Flow rate

Reynolds Number

$$\mathrm{Re} = \frac{\rho \langle v_z \rangle D}{\mu}$$

Pressure Drop

Fanning Friction Factor

$$f = \frac{\frac{1}{4}\left(P_0 - P_L\right)}{\left(\frac{L}{D}\right)\left(\frac{1}{2}\rho \langle v_z \rangle^2\right)}$$

ρ – *density*
$\langle v_z \rangle$ – *average velocity*
D – *pipe diameter*
μ – *viscosity*
$P_0 - P_L$ – *pressure drop*
L – *pipe length*

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Data Correlations for *f*(Re)

Re>4000, turbulent flow:

Prandtl (smooth pipes)	$\frac{1}{\sqrt{f}} = 4\log\left(\mathrm{Re}\sqrt{f}\right) - 0.40$
Colebrook (rough pipes)	$\frac{1}{\sqrt{f}} = -4\log\left(\frac{\varepsilon}{D} + \frac{4.67}{\mathrm{Re}\sqrt{f}}\right) + 2.28$

(Prandtl and Colebrook are equivalent for ε=0)

For Q known, calculate f directly.
For f known, requires iterative calculation of Re.

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Implemented in Excel

given	density=	62.25	lbm/ft3	circular cells
	viscosity=	6.01E-04	lbm/ft.s	
	D=	0.622	in	
	D=	0.052	ft	
	L=	55	ft	
	DeltaP=	60	psi	
	DeltaP=	588	lbf/ft^2	
Step				
1	Flow rate (guess)=	4.60	gpm	
	Flow rate=	0.0102	ft^3/s	
	velocity=	4.8559	ft/s	
2	Re=	26,092		
	guess f=	0.00607		
	RHS Prandtl=	12.83	error=	
3	new_f=	0.00607	0.000%	
4	velocity_second=	4.86	ft/s	
	Q_new=	0.0102	ft^3/s	
5	Q_new=	4.60	gpm	

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Alternative (but more complex) correlation; no iteration on *f* required (F. A. Morrison, 2011)

Flow in smooth pipes: (all Reynolds numbers)

$$f = \left(\frac{0.0076\left(\frac{3170}{Re}\right)^{0.165}}{1+\left(\frac{3170}{Re}\right)^{7.0}} \right) + \frac{16}{Re}$$

(would still need to iterate on Q if used in our problem)

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Analytical Integration of Differential Equations

Solve for *y(x)*: $\frac{dy}{dx} + 2xy = 3x^2 + 1$

Analytical solution (integrating factor):

$$u \equiv 2x$$

$$\int u\, du = \int 2x\, dx = x^2$$

$$e^{\int u\, du} = e^{x^2}$$

$$e^{x^2}\frac{dy}{dx} + e^{x^2}2xy = e^{x^2}\left(3x^2+1\right)$$

$$\frac{d}{dx}\left(e^{x^2}y\right) = e^{x^2}\left(3x^2+1\right)$$

$$e^{x^2}y = \int e^{x^2}\left(3x^2+1\right)dx + C$$

Carry out integral here to obtain final solution for *y(x)*.

$$y = e^{-x^2}\left[\int e^{x^2}\left(3x^2+1\right)dx + C\right]$$

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Numerical Integration of Differential Equations

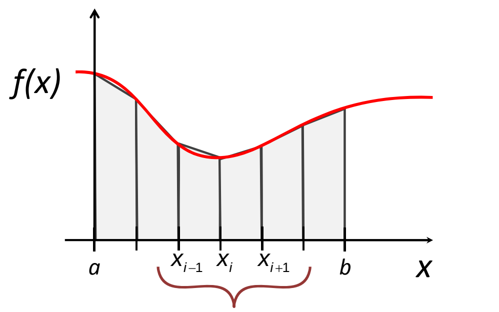
Solve for *y(x)*: $\frac{dy}{dx} + 2xy = 3x^2 + 1$

Before, we were calculating:

$$\frac{dy}{dx} = f(x)$$

$$I = \int_a^b f(x)\,dx$$

and *f(x)* was known. In the current calculation, our integration is not explicitly *dy/dx=f(x)*



In the trapezoidal rule integration, we discretized *x*, evaluated *f(x)*, and summed areas.

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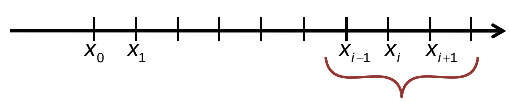
Numerical Integration of Differential Equations

Solve for y: $\frac{dy}{dx} + 2xy = 3x^2 + 1$

We can discretize the current differential equation as well:

$$\frac{dy_i}{dx_i} + 2x_i y_i = 3x_i^2 + 1$$



$$y_i = \frac{1}{2x_i}\left(3x_i^2 + 1 - \frac{dy_i}{dx_i}\right)$$

where to get this at each step?

Strategy: Develop efficient and accurate algorithms that allow us to calculate *y(x)* and its derivatives at a location *(i+1)* from knowledge of *y(x)* at neighboring locations *(i)*, *(i-1)*, etc.

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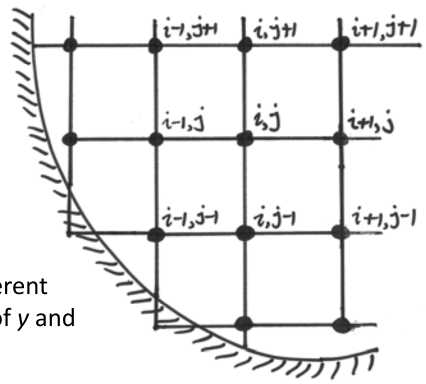
Numerical Integration of Differential Equations

In two dimensions (or three), the discretization system is called the mesh.



Algorithms:
- Finite difference
- Finite elements
- Finite volumes
- Etc.

Different algorithms use different logic to estimate the values of y and derivatives of y at different locations.

Numerical integration of differential equations has a long history that predates computers. . .

Reference:
Numerical Methods Using Mathcad,
Laurene Fausett, Prentice Hall, 2002

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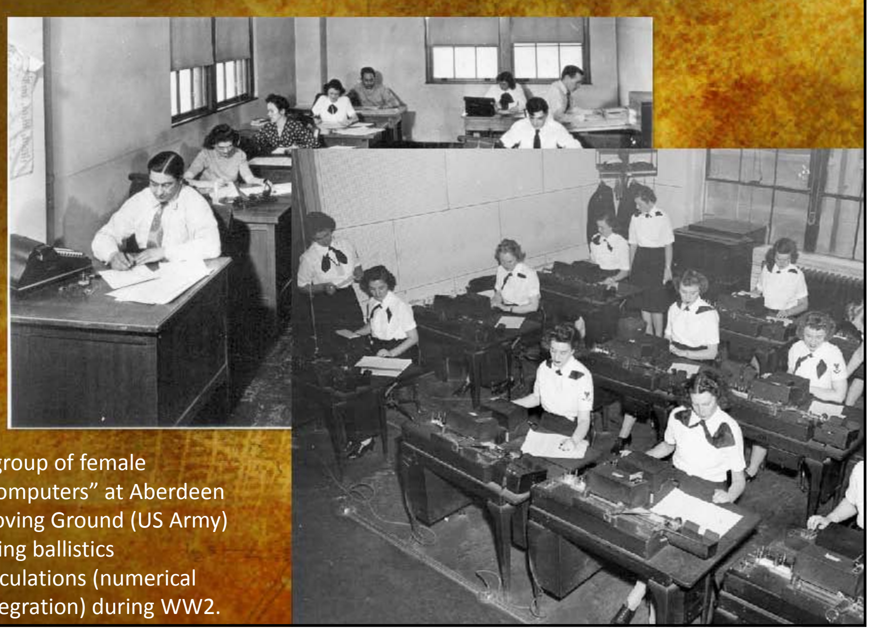
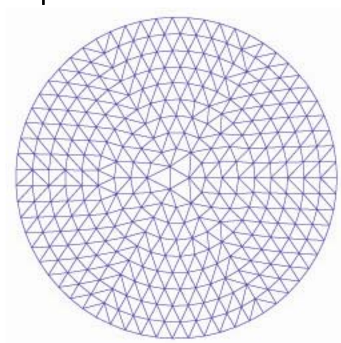
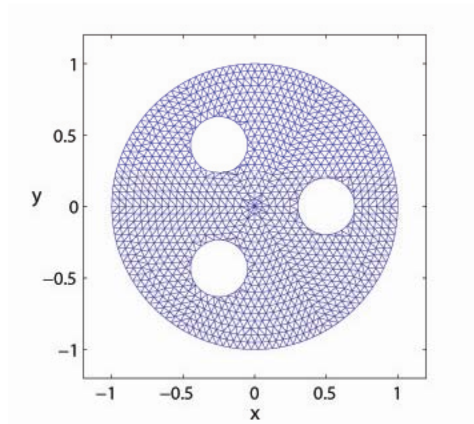
From "ENIAC, Human Computing and the Top Secret Rosies of WWII," PPT accompanying the documentary Top Secret Rosies, www.topsecretrosies.c



A group of female "Computers" at Aberdeen Proving Ground (US Army) doing ballistics calculations (numerical integration) during WW2.

Meshes for Numerical Integration of Differential Equations





The discretization (mesh) is chosen to minimize the effect of numerical errors and modeling approximations on the final results.

Provided by Dr. Tom Co, 2011

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Issues affecting accuracy of solutions of flow problems using the Navier-Stokes equation

Analytical Solutions are affected by **BOTH** Numerical Solutions are affected by

Continuum hypothesis

Symmetry assumptions

Approximate geometry

Approximate boundary conditions

Steady state assumption

Incompressible fluid

Newtonian fluid

Isothermal, single-phase flow

Finite domain size

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Issues affecting accuracy of solutions of flow problems using the Navier-Stokes equation

Analytical Solutions are affected by	Numerical Solutions are affected by
Neglect inconvenient terms	Discretization of flow domain
Linearization and other approximate analytical solution methods	Derivative approximations
Final solution series truncation error	Round-off error
	Interpolation error in final engineering quantities
	Numerical instability induced by accumulation of error
	Inappropriate implementation of commercial code

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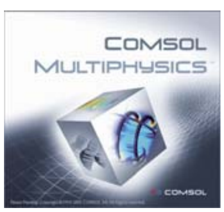
Numerical PDE Solving with Comsol 4.2



www.comsol.com

Finite-element numerical differential equation solver. Applications include fluid mechanics and heat transfer.

1. Choose the physics (2D, 2D axisymmetric, laminar, steady/unsteady, etc.)
2. Choose flow geometry and fluid (shape of the flow domain)
3. Define boundary conditions
4. Design and generate mesh
5. Solve the problem
6. Calculate and plot engineering quantities of interest.

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Comsol Multiphysics 4.2

Launch the program **0**

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Comsol Multiphysics 4.2

Launch the program **0**

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Comsol Multiphysics 4.2

Launch the program

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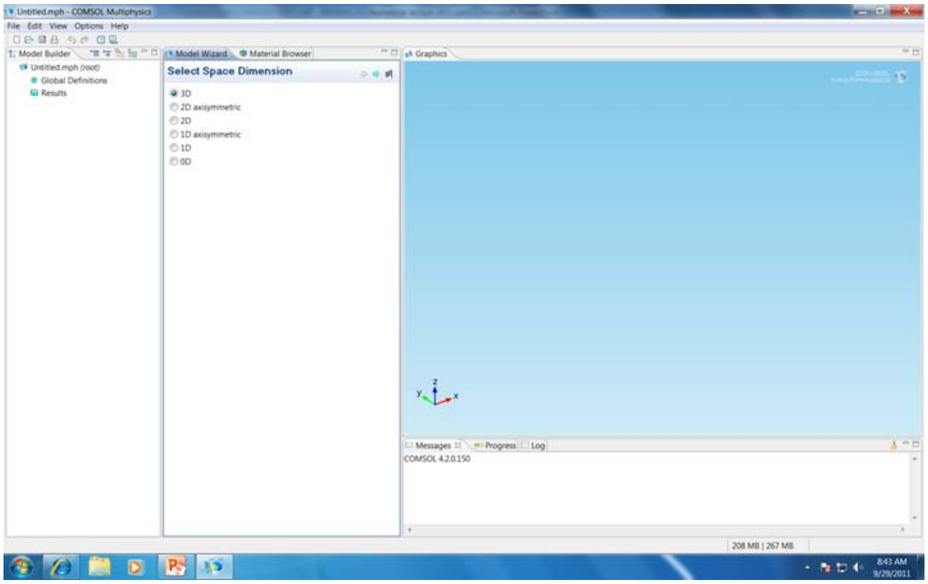

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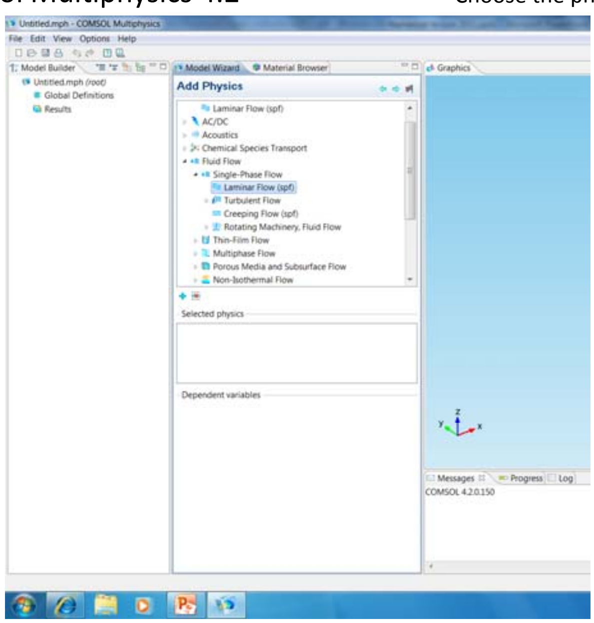
Comsol Multiphysics 4.2

Choose the physics

1



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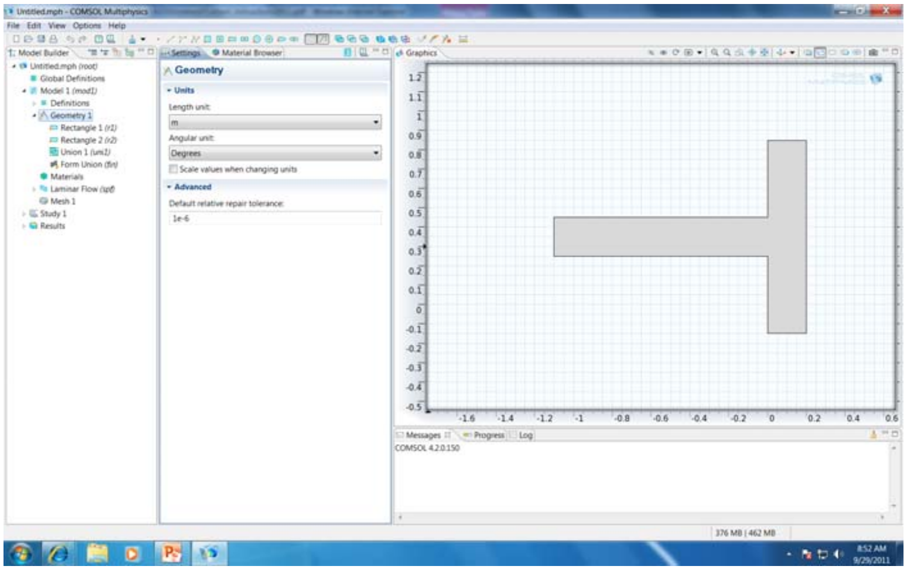
Choose flow geometry and fluid **2**



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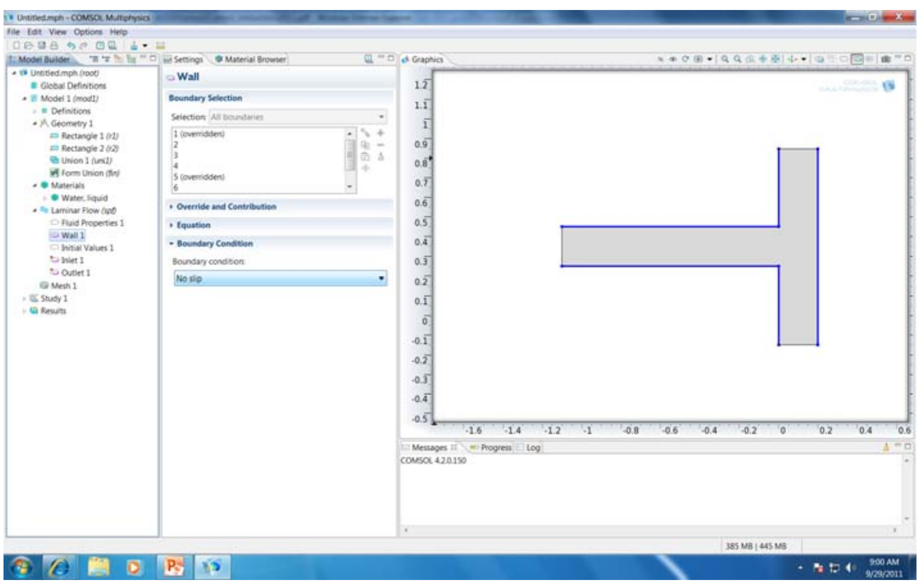
Comsol Multiphysics 4.2

Define boundary conditions **3**



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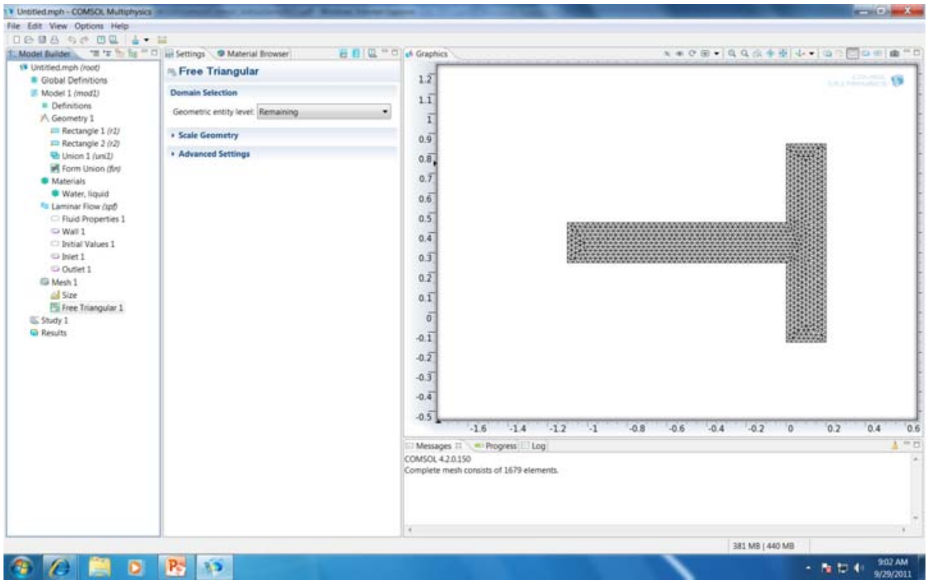
Design and generate mesh

4



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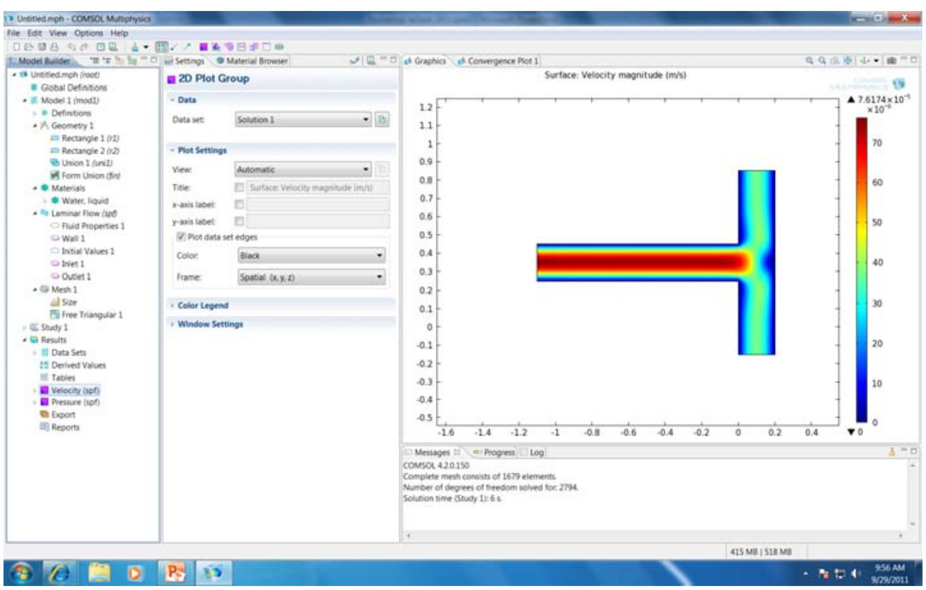
Comsol Multiphysics 4.2

Solve the problem

5



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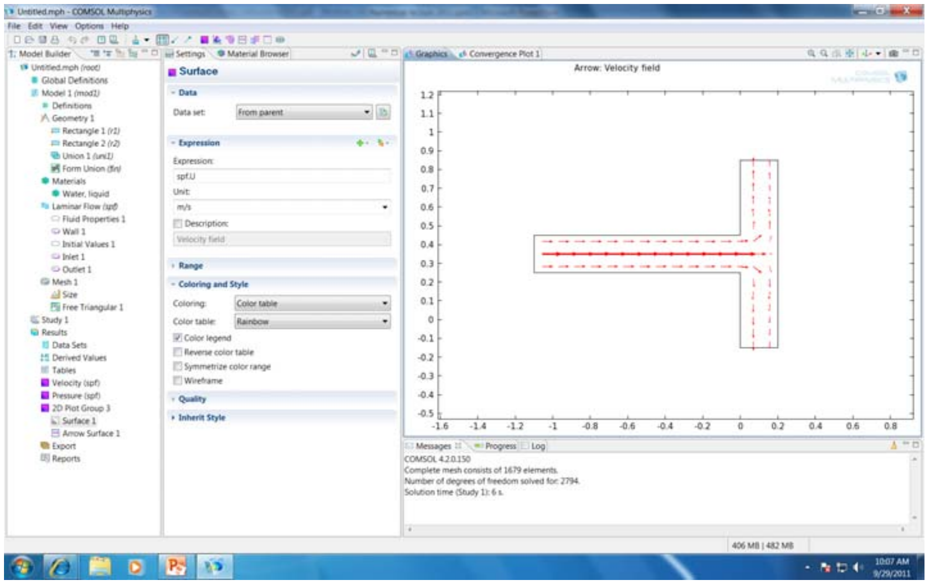
Comsol Multiphysics 4.2

View the solution **5**



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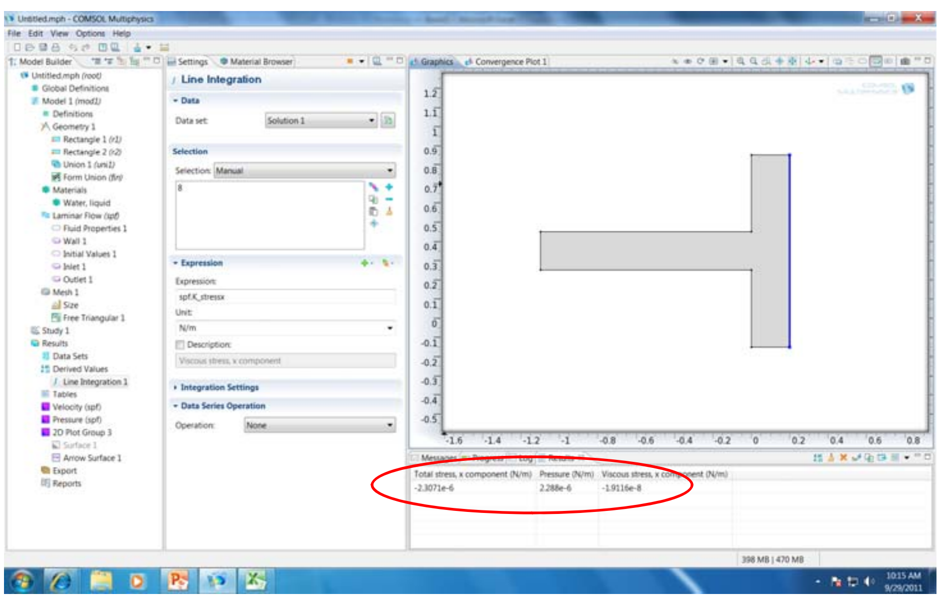
Comsol Multiphysics 4.2

Calculate engineering problems of interest **6**



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***SUMMARY:** Numerical methods in transport phenomena/chemical engineering*

MichiganTech

Calculators can do numerical integration of the problem is a once-and-done sort

•Numerical integration (one-dimensional; trapezoidal rule)

•Optimization (Excel Solver)

Great for model fitting

•Iterative Problem Solving

•Numerical integration (two-dimensional; finite-element package Comsol)

Programmable calculators can do iterative calculations if it is a once-and-done sort

State of the art for complex geometries in many fields

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