

Optimal Design of Energy Systems

Chapter 6 System Simulation

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Chapter 6. System Simulation

6.1 Introduction

calculation of operating variables

[characteristics of all components
thermodynamic properties

→ a set of simultaneous equations



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6.2 Some use of simulation

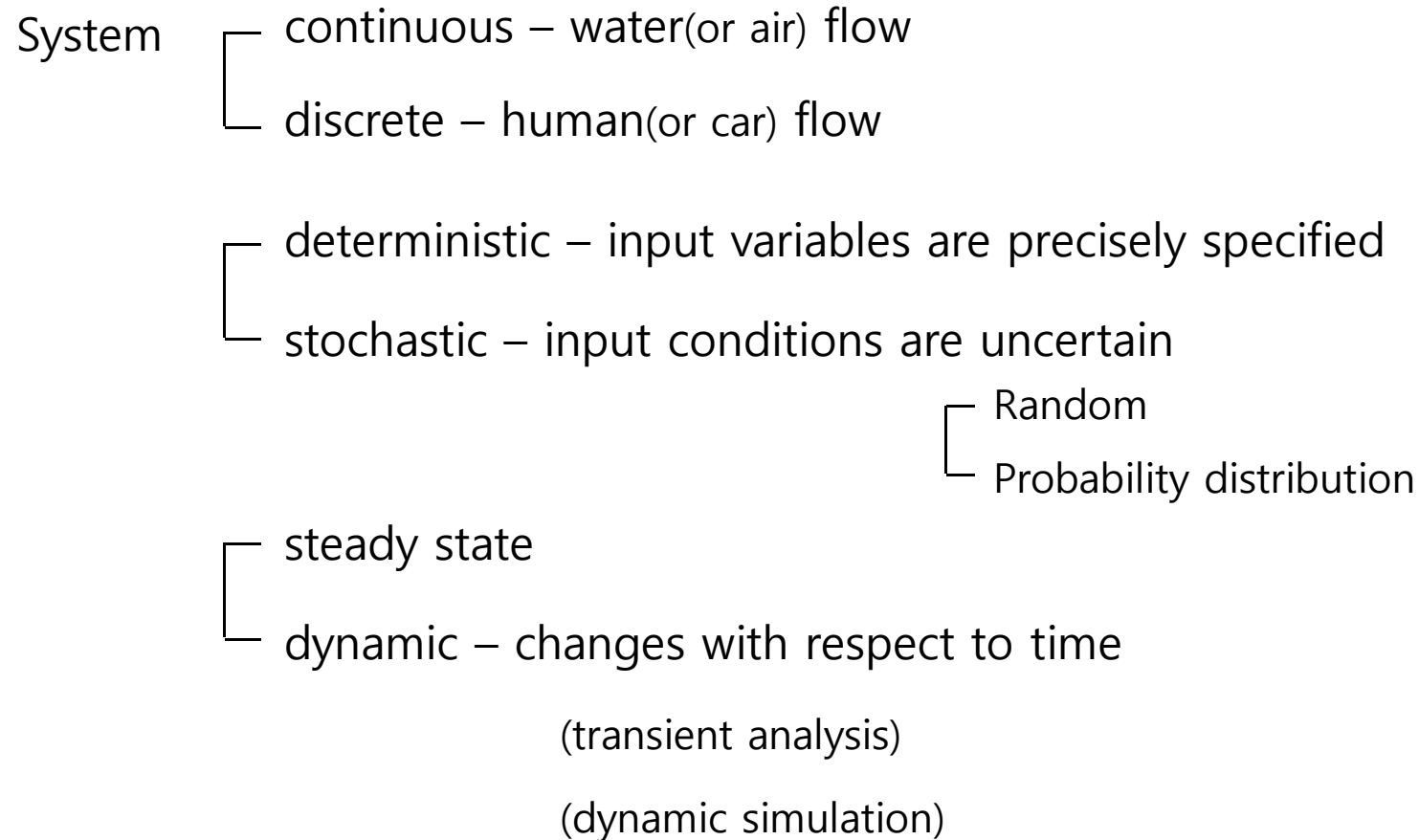
- ┌ Design stage – to achieve improved design
- └ Existing system – to explore prospective modifications
(operating stage)

- ┌ Design condition
- └ Off design condition (part load / over load) ← normal operation



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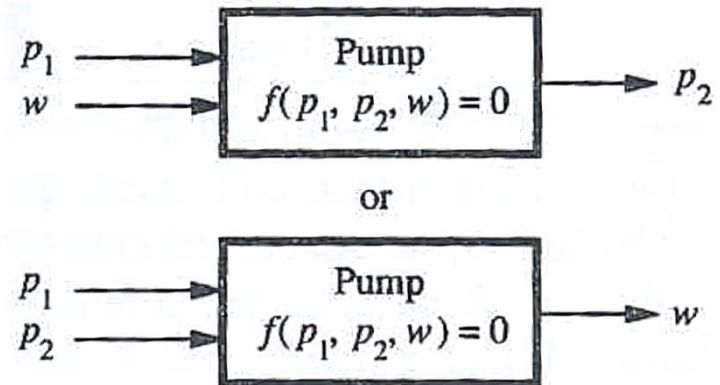
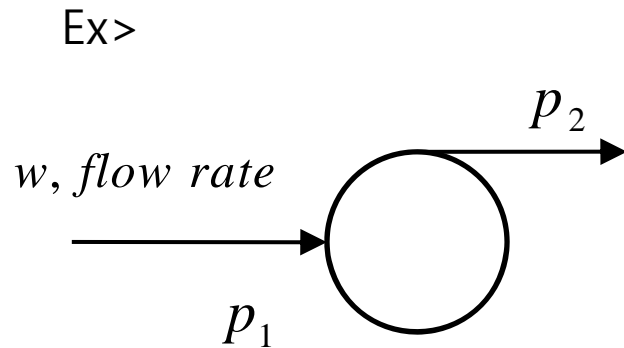
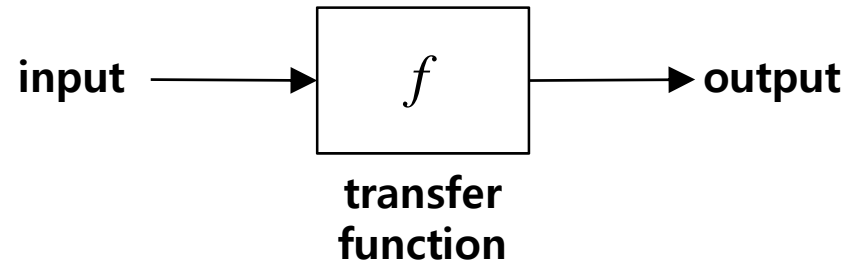
6.3 Classes of simulation



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6.4 Information Flow diagram

[Fluid
 [Energy



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6.4 Information Flow diagram

$$w_A = C_A \sqrt{p_3 - p_{atm}}$$

$$w_B = C_B \sqrt{p_4 - p_{atm}}$$

$$P_2 - P_3 = C_2 w_1^2$$

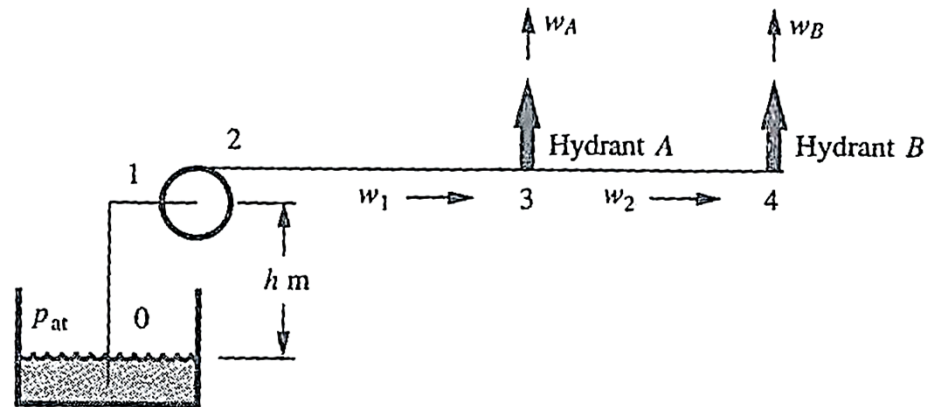
$$P_3 - P_4 = C_3 w_2^2$$

$$p_{atm} = p_1 + C_2 w_1^2 + \rho g h$$

pump $w_1 = f(p_1, p_2)$

mass balance $w_1 = w_A + w_2$

$$w_2 = w_B$$



of equations = 8

of variables = 8



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6.4 Information Flow diagram

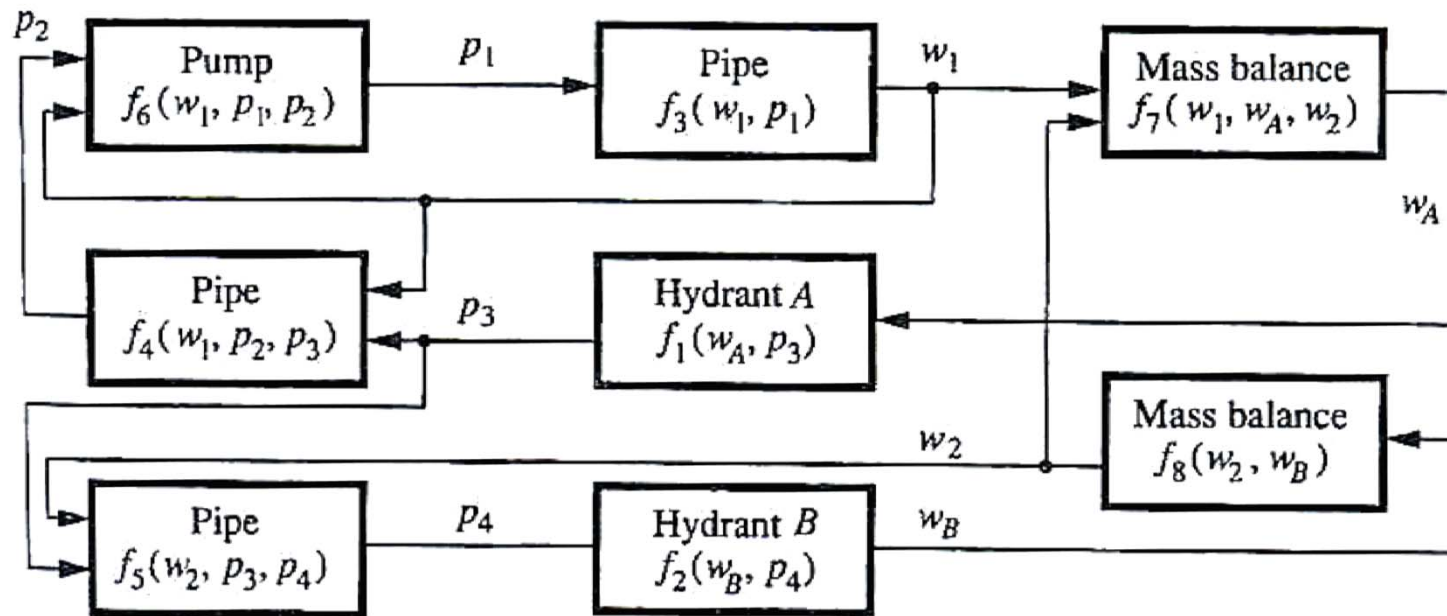


FIGURE 6-3
Information-flow diagram for fire-water system.

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6.6 Two methods of simulation

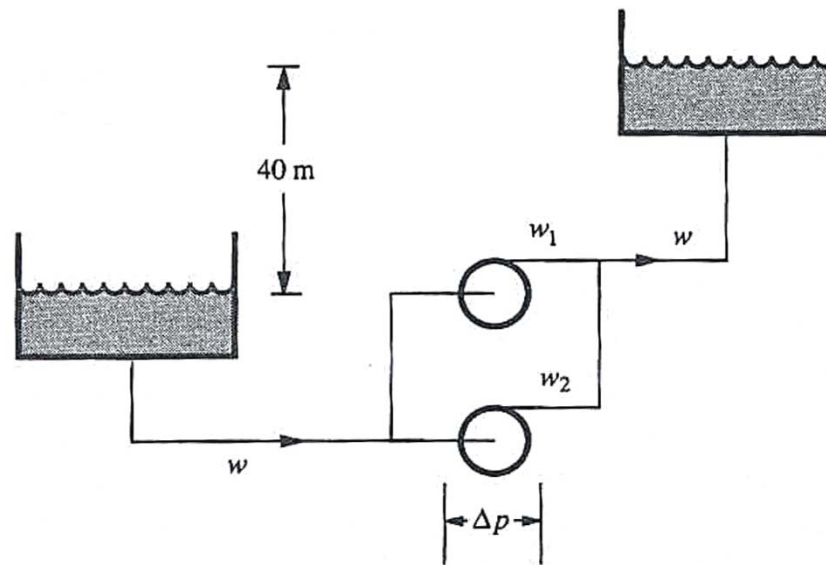
- Successive substitution
- Newton-Raphson



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6.7 Successive substitution

<Example 6.1> What are w_1 , w_2 , w and ΔP ?



- Pump 1 : $\Delta p = 810 - 25w_1 - 3.75w_1^2$
- Pump 2 : $\Delta p = 900 - 65w_2 - 30w_2^2$



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6.7 Successive substitution

<Solution>

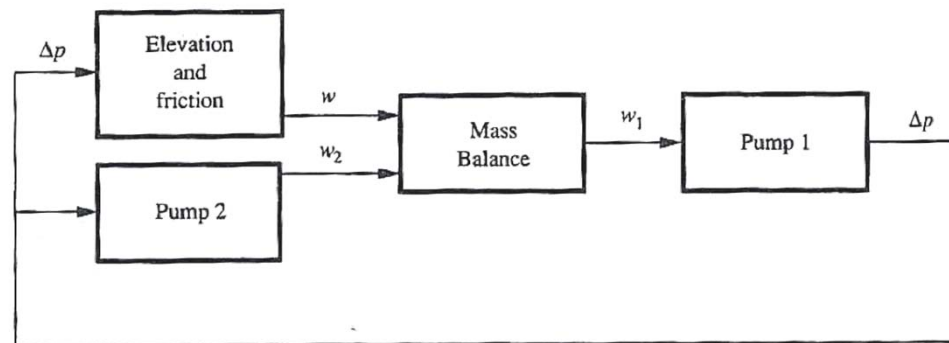
- ✓ Pressure difference due to elevation and friction :

$$\Delta p = 7.2w^2 + \frac{(40 \text{ m})(1000 \text{ kg / m}^3)(9.807 \text{ m / s}^2)}{1000 \text{ Pa / kPa}}$$

- ✓ Pump 1 : $\Delta p = 810 - 25w_1 - 3.75w_1^2$

- ✓ Pump 2 : $\Delta p = 900 - 65w_2 - 30w_2^2$

- ✓ Mass balance : $w = w_1 + w_2$

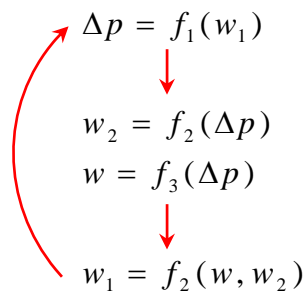


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6.7 Successive substitution

<Solution>

- ✓ Iteration with initial assumption : $w_1 = 4.2$



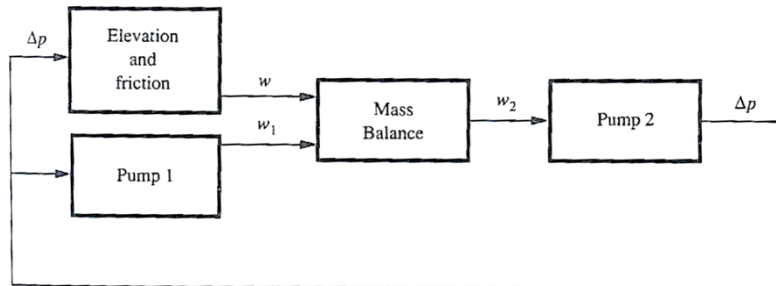
Iteration	w_1 [kg/s]	w_2 [kg/s]	w [kg/s]	Δp [kPa]
1	<u>4.200</u>	2.060	5.852	638.85
2	3.792	1.939	6.112	661.26
3	4.174	2.052	5.870	640.34
4	3.818	1.946	6.097	659.90
5	4.151	2.045	5.885	641.63
⋮	⋮	⋮	⋮	⋮
∞	3.991	1.997	5.988	650.49



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6.8 Pitfalls in successive substitution

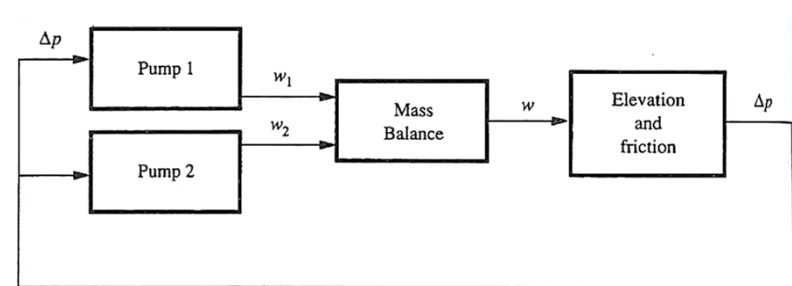
Diagram 2



Iteration	w_1 [kg/s]	w_2 [kg/s]	w [kg/s]	Δp [kPa]
1	4.000	2.000	5.983	650.00
2	3.942	1.983	6.019	653.16
3	4.258	2.077	5.812	635.53
4	2.443	1.554	6.814	726.54
5	11.353	4.371	divergence	42.87

✓ Divergence occurs

Diagram 3



Iteration	w_1 [kg/s]	w_2 [kg/s]	w [kg/s]	Δp [kPa]
1	3.973	1.992	6.000	651.48
2	4.028	2.008	5.965	648.47
3	3.916	1.975	6.036	654.61
⋮	⋮	⋮	⋮	⋮
9	divergence		8.811	951.23

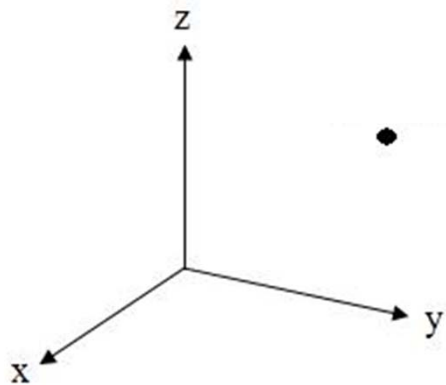
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6.9 Taylor series expansion

$$z = z(x, y)$$

Near the point $(a, b, z(a, b))$

$$z = c_0 + c_1(x - a) + c_2(y - b) + c_3(x - a)^2 + c_4(x - a)(y - b) + c_5(y - b)^2 + \dots$$



$$c_0 = z(a, b)$$

$$c_1 = \frac{\partial z(a, b)}{\partial x}$$

$$c_2 = \frac{\partial z(a, b)}{\partial y}$$

$$c_3 = \frac{1}{2} \frac{\partial^2 z(a, b)}{\partial x^2}$$

$$c_4 = \frac{\partial^2 z(a, b)}{\partial x \partial y}$$

$$c_5 = \frac{1}{2} \frac{\partial^2 z(a, b)}{\partial y^2}$$



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6.9 Taylor series expansion

- $y = y(x)$

$$y = d_0 + d_1(x - a) + d_2(x - a)^2 + \dots$$

$$d_0 = y(a) \quad d_1 = \frac{dy(a)}{dx} \quad d_2 = \frac{1}{2} \frac{d^2 y(a)}{dx^2}$$

- $y = y(x_1, x_2, \dots, x_n)$

$$\begin{aligned} y &= y(a_1, a_2, \dots, a_n) + \sum_{j=1}^n \frac{\partial y(a_1, a_2, \dots, a_n)}{\partial x_j} (x_j - a_j) \\ &+ \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \frac{\partial^2 y(a_1, a_2, \dots, a_n)}{\partial x_i \partial x_j} (x_j - a_i)(x_j - a_j) \\ &+ \dots \end{aligned}$$



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6.9 Taylor series expansion

<Example 6.2> Express $z = \ln(x^2 / y)$ as a Taylor-series expansion at $(x=2, y=1)$

<Solution>

$$z = \ln \frac{x^2}{y} = c_0 + c_1(x - 2) + c_2(y - 1) + c_3(x - 2)^2 + c_4(x - 2)(y - 1) + c_5(y - 1)^2 + \dots$$

$$c_0 = \ln \frac{2^2}{1} = 1.39$$

$$c_3 = \frac{1}{2} \frac{\partial^2 z(2,1)}{\partial x^2} = \frac{1}{2} \left(-\frac{2}{x^2} \right) = -\frac{1}{4}$$

$$c_1 = \frac{\partial z(2,1)}{\partial x} = \frac{2x/y}{x^2/y} = 1$$

$$c_4 = \frac{\partial^2 z(2,1)}{\partial x \partial y} = 0$$

$$c_2 = \frac{\partial z(2,1)}{\partial y} = -\frac{x^2/y^2}{x^2/y} = -1$$

$$c_5 = \frac{1}{2} \frac{\partial^2 z(2,1)}{\partial y^2} = \frac{1}{2} \frac{1}{y^2} = \frac{1}{2}$$

$$\therefore z = 1.39 + (x - 2) - (y - 1) - \left(\frac{1}{4}\right)(x - 2)^2 + \left(\frac{1}{2}\right)(y - 1)^2 + \dots$$

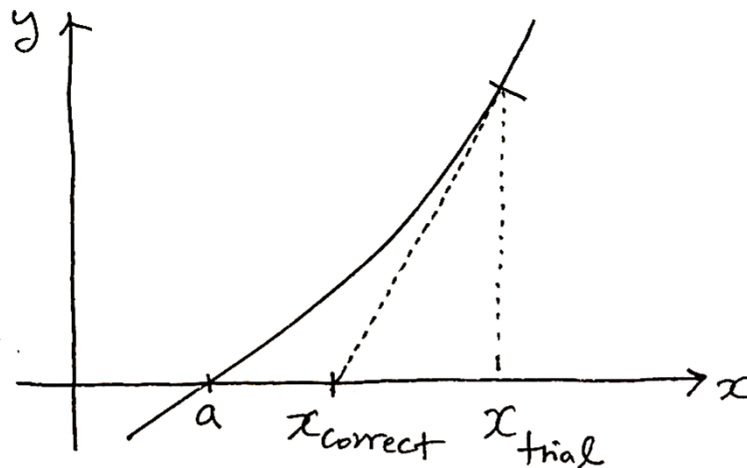


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6.10 Newton-Raphson with one equation and one unknown

$$y = y(x) \quad x \approx a$$

$$\rightarrow y(x) \approx y(a) + y'(a)(x - a)$$



$$y(x_t) = y(x_c) + \frac{y(x_t) - y(x_c)}{x_t - x_c} (x_t - x_c)$$

$$x_c = x_t - \frac{y(x_t)}{y'(x_t)}$$

$$x_{new} = x_{old} - (x_{trial} - x_{correct})$$



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6.10 Newton-Raphson with one equation and one unknown

Ex> $y(x) = x + 2 - e^x$, $y(x_c) = 0$

if $x_t = 2$ $y(x_t) = x_t + 2 - e^{x_t} = -3.39$

$$x_c = 2 - \frac{-3.39}{1 - e^2} = 1.469 \rightarrow x_{t,new}$$

Iteration	x_t	$y(x)$	$y'(x)$	x_c
1	2.000	-3.389	-6.389	1.470
2	1.470	-0.878	-3.347	1.207
3	1.207	-0.137	-2.345	1.149
4	1.149	-0.006	-2.154	1.146
5	1.146	0.000	-2.146	



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6.11 Newton-Raphson with multiple equations and unknowns

$$f_1(x_1, x_2, x_3) = 0$$

$$f_2(x_1, x_2, x_3) = 0$$

$$f_3(x_1, x_2, x_3) = 0$$

trial value : x_{1t}, x_{2t}, x_{3t}

$$\begin{aligned} f_1(x_{1t}, x_{2t}, x_{3t}) &= f_1(x_{1c}, x_{2c}, x_{3c}) + \frac{\partial f_1(x_{1t}, x_{2t}, x_{3t})}{\partial x_1} (x_{1t} - x_{1c}) \\ f_2 &= \dots + \frac{\partial f_1(x_{1t}, x_{2t}, x_{3t})}{\partial x_2} (x_{2t} - x_{2c}) \\ f_3 &= \dots + \frac{\partial f_1(x_{1t}, x_{2t}, x_{3t})}{\partial x_3} (x_{3t} - x_{3c}) \\ &+ \dots \end{aligned}$$



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6.11 Newton-Raphson with multiple equations and unknowns

$$\begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \\ \frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} \end{bmatrix} \begin{bmatrix} x_{1t} - x_{1c} \\ x_{2t} - x_{2c} \\ x_{3t} - x_{3c} \end{bmatrix} = \begin{bmatrix} f_1(x_{1t}, x_{2t}, x_{3t}) \\ f_2(x_{1t}, x_{2t}, x_{3t}) \\ f_3(x_{1t}, x_{2t}, x_{3t}) \end{bmatrix}$$

$$\rightarrow x_{i,new} = x_{i,old} - (x_{i,t} - x_{i,c})$$



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6.11 Newton-Raphson with multiple equations and unknowns

<Example 6.3> Solve Example 6.1 by Newton-Raphson method

<Solution>

✓ requirement : $f_1 = \Delta p - 7.2w^2 - 392.28 = 0$

$$f_2 = \Delta p - 810 + 25w_1 + 3.75w_1^2 = 0$$

$$f_3 = \Delta p - 900 + 65w_2 + 30w_2^2 = 0$$

$$f_4 = w - w_1 + w_2 = 0$$

✓ trial value : $\Delta p = 750, w_1 = 3, w_2 = 1.5, w = 5$

$$\rightarrow f_1 = 177.7, f_2 = 48.75, f_3 = 15.0, f_4 = 0.50$$

	$\partial/\partial\Delta p$	$\partial/\partial w_1$	$\partial/\partial w_2$	$\partial/\partial w$
$\partial f_1/\partial$	1	0	0	-14.4w
$\partial f_2/\partial$	1	25+7.5w ₁	0	0
$\partial f_3/\partial$	1	0	65+60w ₂	0
$\partial f_4/\partial$	0	-1	-1	1



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6.11 Newton-Raphson with multiple equations and unknowns

<Solution>

$$\checkmark \begin{bmatrix} 1.0 & 0.0 & 0.0 & -72.0 \\ 1.0 & 47.5 & 0.0 & 0.0 \\ 1.0 & 0.0 & 155.0 & 0.0 \\ 0.0 & -1.0 & -1.0 & 1.0 \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \Delta x_3 \\ \Delta x_4 \end{bmatrix} = \begin{bmatrix} 177.7 \\ 48.75 \\ 15.0 \\ 0.50 \end{bmatrix} \quad \Delta x_i = x_{i,t} - x_{i,c}$$

$$\checkmark \Delta x_1 = 98.84, \Delta x_2 = -1.055, \Delta x_3 = -0.541, \Delta x_4 = -1.096$$

$$\checkmark \text{corrected variable : } \Delta p = 750 - 98.84 = 651.16, w_1 = 4.055, w_2 = 2.041, w = 6.096$$

Iteration	w_1 [kg/s]	w_2 [kg/s]	w [kg/s]	Δp [kPa]	f_1	f_2	f_3	f_4
1	3.000	1.500	5.000	750.00	177.720	48.750	15.000	0.500
2	4.055	2.041	6.096	651.16	-8.641	4.171	8.778	0.000
3	3.992	1.998	5.989	650.48	-0.081	0.015	0.056	0.000
4	<u>3.991</u>	<u>1.997</u>	<u>5.988</u>	<u>650.49</u>	0.000	0.000	0.000	0.000

$$\therefore \Delta p = 650.49, w_1 = 3.991, w_2 = 1.997, w = 5.988$$

