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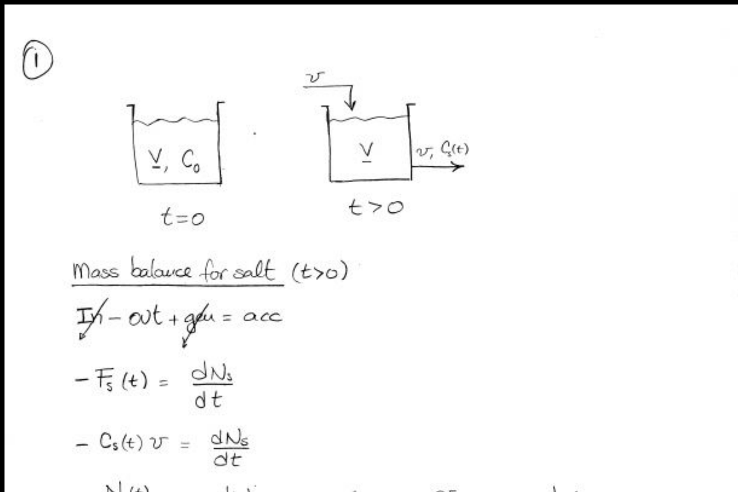
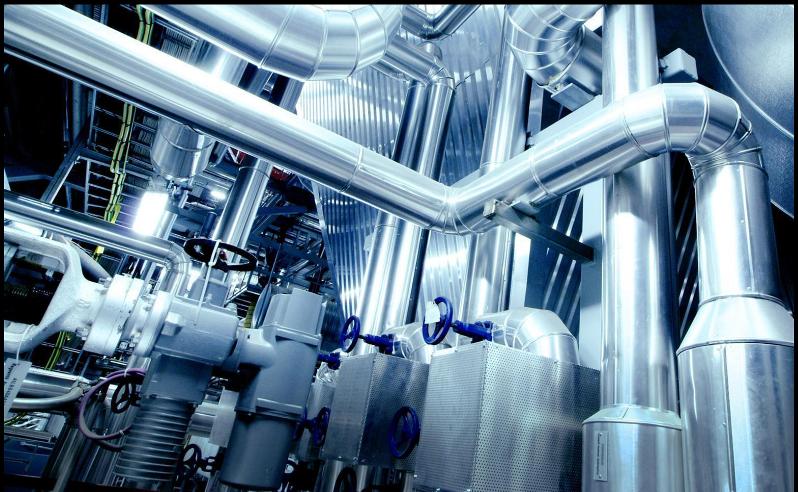




ChE352

Numerical Techniques for Chemical Engineers

Professor Stevenson

Lecture 11

Recall: IVP Systems in Python

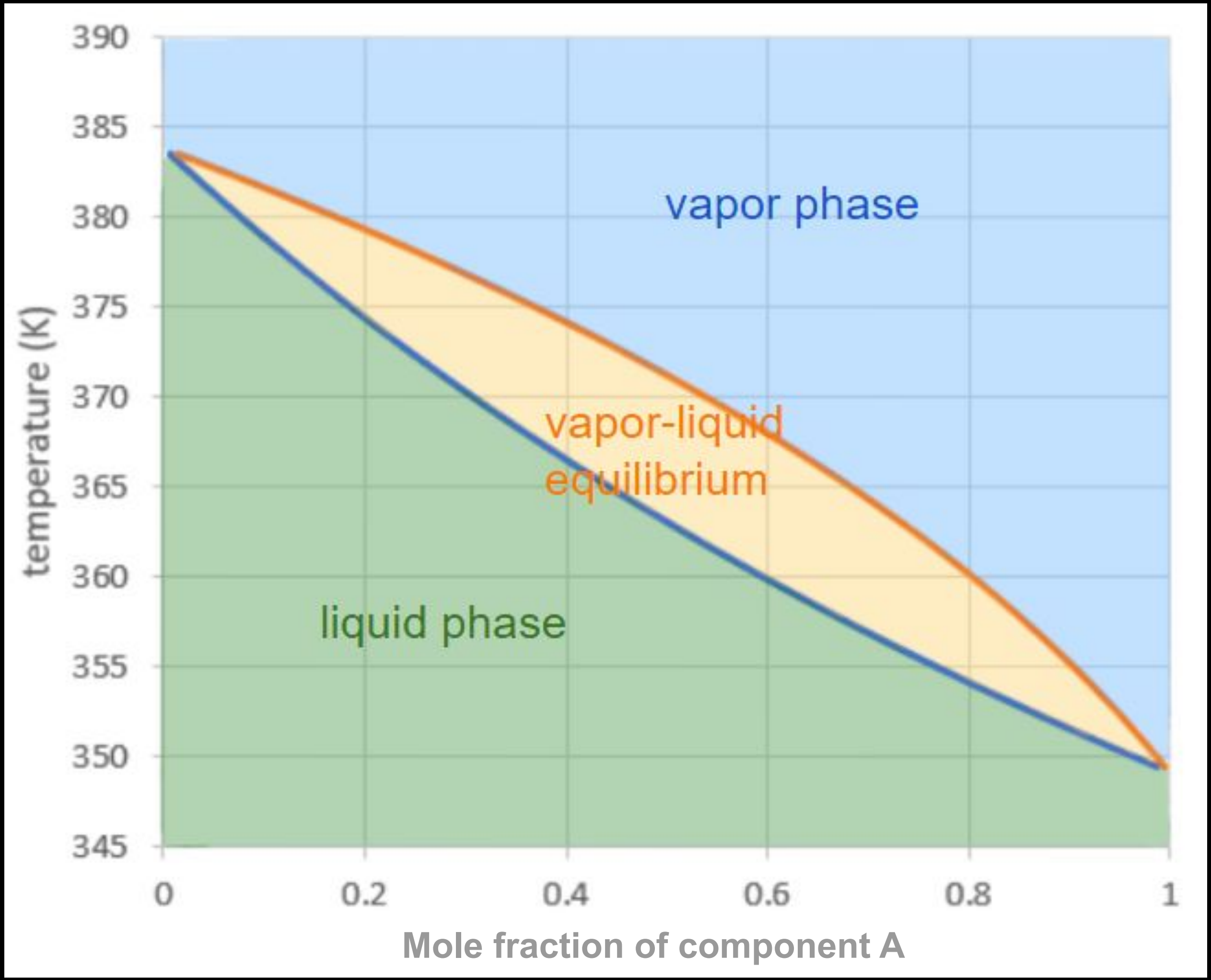
```
from scipy.integrate import solve_ivp
def fun(t, u):  # 3-D IVP
    C_A, C_B, C_C = u
    ... calculate derivatives here ...
    return dAdt, dBdt, dCdt
sol = solve_ivp(fun, (t0, t_final), u0)
plt.plot(sol.t, sol.y[0], label='[A]')
plt.plot(sol.t, sol.y[1], label='[B]')
plt.plot(sol.t, sol.y[2], label='[C]')
```

n-Dimensional "Well-Posed" IVPs

- If all of the following are true, the <u>IVP system</u> is <u>well-posed</u> (unique solution, bounded error with respect to changes in f):
- f must be a vector function & continuous
  - What is a vector function? How is it continuous?
- All the partial first derivatives of f must be continuous in all dimensions (t, u_1, u_2, etc.)
- u and t must live in <u>convex spaces</u>
  - For any two points (t_1, u_1) & (t_2, u_2), all points on the line between them are also valid for the IVP
  - Example non-convex space: IVP of volatile liquids

Non-convex example IVP

- Imagine solving an IVP for a reaction A→B as a liquid
- Want C_A and T
- Between some good C_A and T, you can draw a line where VLE is present (so you need P too)



Non-convex example IVP

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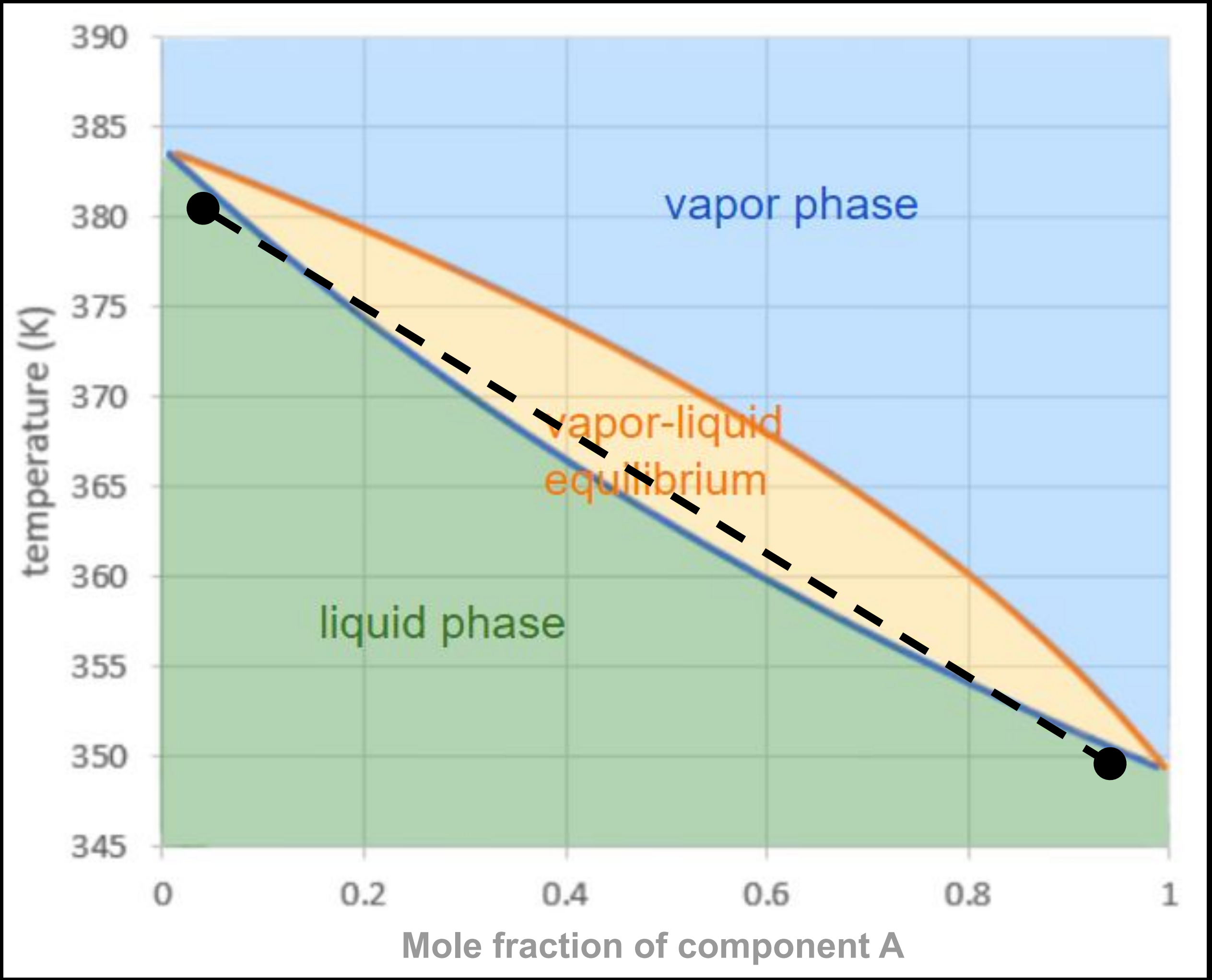
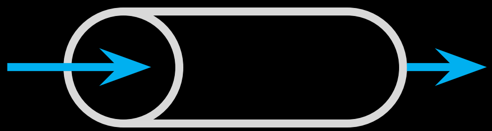


Activity: define an IVP system

$$2A \xrightarrow{k_1} B \xrightarrow{k_2} C$$



$$\frac{dC_A}{dz} = -2k_1 C_A^{\,2}, \quad C_A(z=0) = C_A^o$$

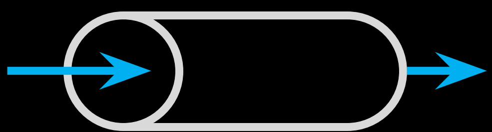
$$\frac{dC_B}{dz} = -k_2 C_B + k_1 C_A^{\,2}, \quad C_B(z=0) = 0$$

$$\frac{dC_C}{dz} = k_2 C_B, \quad C_C(z=0) = 0$$

Put this system, two sequential reactions with three species, into the general form for an IVP system by stating t, u, and f(t, u). Also state the initial conditions. How might we pick t_{end}?

Activity: define an IVP system

$$2A \xrightarrow{k_1} B \xrightarrow{k_2} C$$



$$\frac{dC_A}{dz} = -2k_1 C_A^{\,2}, \quad C_A(z=0) = C_A^o$$

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$$\frac{dC_C}{dz} = k_2 C_B, \quad C_C(z=0) = 0$$

$$\boxed{t = z} \quad u_1(t) = C_A(z), \quad u_2(t) = C_B(z), \quad u_3(t) = C_C(z)$$

$$\boxed{u = \begin{bmatrix} C_A & C_B & C_C \end{bmatrix}^T}$$

Choice of t_{end} depends on whether you're *modeling* or *designing*

Answer: define an IVP system

$$\boxed{t = z} \quad u_1(t) = C_A(z), \quad u_2(t) = C_B(z), \quad u_3(t) = C_C(z)$$

$$\boxed{u = \begin{bmatrix} C_A & C_B & C_C \end{bmatrix}^T}$$

Can define f(t, u) to give a single vector or multiple scalars (same thing)

$$f_1(t,u) = -2k_1 C_A{}^2 = -2k_1 u_1{}^2$$

$$f_2(t,u) = -k_2 C_B + k_1 C_A{}^2 = -k_2 u_2 + k_1 u_1{}^2$$

$$f_3(t,u) = k_2 C_B = k_2 u_2$$

$$\boxed{f(t,u) = \begin{bmatrix} -2k_1 u_1{}^2 & -k_2 u_2 + k_1 u_1{}^2 & k_2 u_2 \end{bmatrix}^T}$$

$$\boxed{t_0 = 0} \qquad \boxed{a = \begin{bmatrix} C_A^o & 0 & 0 \end{bmatrix}^T}$$

Vector function f(t, u) maps R^4 onto R^3.

What does this mean?

Activity: Euler for IVP systems

$\boxed{t = z}$ $\quad u_1(t) = C_A(z), \quad u_2(t) = C_B(z), \quad u_3(t) = C_C(z)$

$\boxed{u = \begin{bmatrix} C_A & C_B & C_C \end{bmatrix}^T}$

Define the <u>Euler step</u> for this system in terms of step size h

$$f_1(t,u) = -2k_1 C_A{}^2 = -2k_1 u_1{}^2$$

$$f_2(t,u) = -k_2 C_B + k_1 C_A{}^2 = -k_2 u_2 + k_1 u_1{}^2$$

$$f_3(t,u) = k_2 C_B = k_2 u_2$$

$$\boxed{f(t,u) = \begin{bmatrix} -2k_1 u_1{}^2 & -k_2 u_2 + k_1 u_1{}^2 & k_2 u_2 \end{bmatrix}^T}$$

$\boxed{t_0 = 0}$ $\quad \boxed{a = \begin{bmatrix} C_A^o & 0 & 0 \end{bmatrix}^T}$

(Remember, an Euler step is purely linear)

Answer: Euler for IVP systems

f(t, u) for this IVP: $\boxed{f(t,u) = \begin{bmatrix} -2k_1u_1^2 & -k_2u_2 + k_1u_1^2 & k_2u_2 \end{bmatrix}^T}$

Euler step in general: $w_{i,j+1} = w_{i,j} + hf(t_j, w_{i,j})$

Euler step for this IVP:

$$w_{1,j+1} = w_{1,j} + h(-2k_1w_{1,j}^2)$$

$$w_{2,j+1} = w_{2,j} + h(-k_2w_{2,j} + k_1w_{1,j}^2)$$

$$w_{3,j+1} = w_{3,j} + hk_2w_{2,j}$$

Euler's Method for multiple dimensions is almost identical to Euler's Method in one dimension

Recall: RK methods in 1D

- RK methods use Δt, Δy, and f(t+Δt, y+Δy) to approximate the curvature of y, permit better than linear (aka better than Euler) steps
  - How are derivatives of f(t, y) related to curvature?

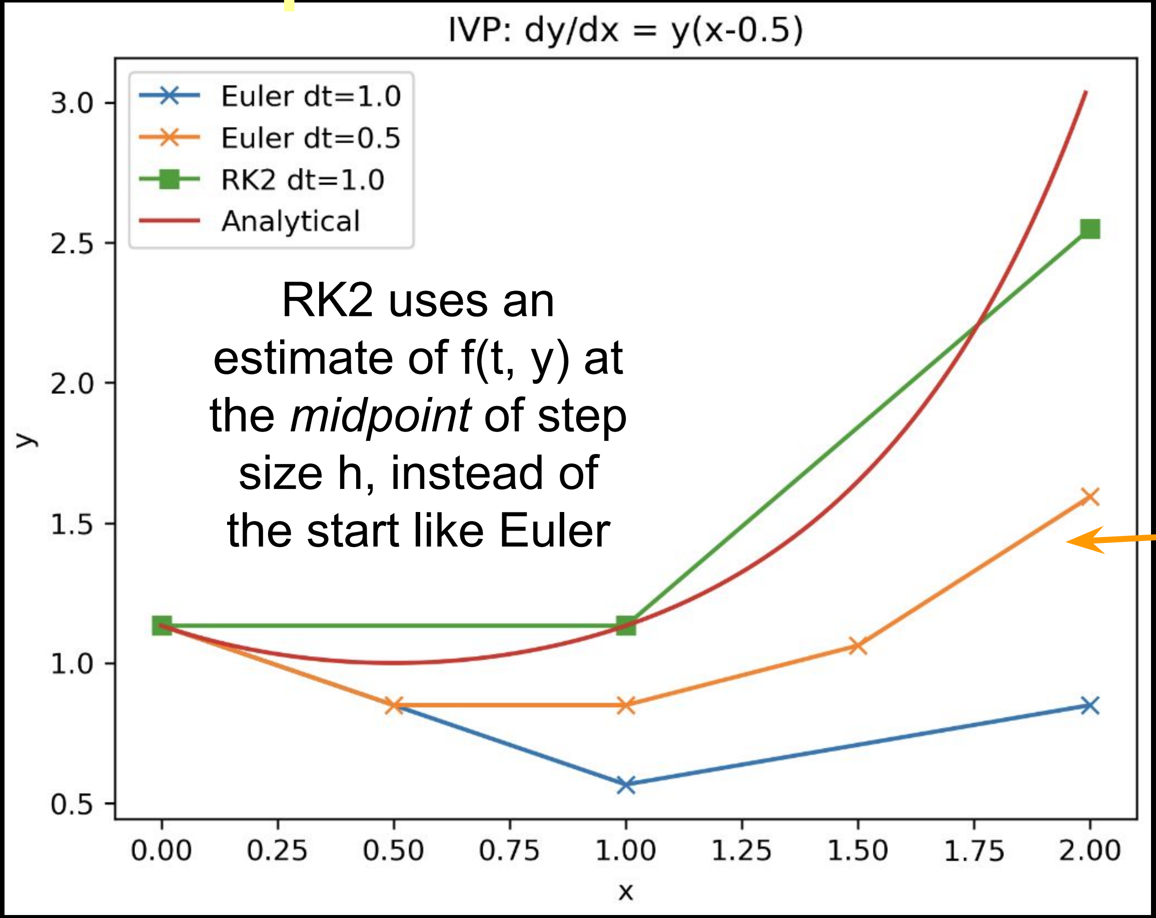
$$hf\left(t_i+\Delta t, y(t_i)+\Delta y\right) \approx \boxed{h\left[f\left(t_i, y(t_i)\right)\right.} + \boxed{\left.\Delta t\left(\frac{\partial f}{\partial t}\right)_{t_i, y(t_i)} + \Delta y\left(\frac{\partial f}{\partial y}\right)_{t_i, y(t_i)}\right]}$$

- If we calculate f' numerically, we get this nested expression known as RK2:

$$\boxed{w_{i+1} = w_i + h\left[\boxed{f\left(t_i+\frac{h}{2}, w_i+\boxed{\frac{h}{2}f\left(t_i, w_i\right)}\right)}\right]}$$

Example: Euler vs RK2

Note the *curvature* of the function y(t). This is what makes an IVP hard for Euler's Method.



Even with twice as many steps, so both call f(t,y) equally, Euler can't catch up with RK2 here.

$$w_{i+1} = w_i + h\left[\boxed{f\left(t_i+\frac{h}{2}, w_i + \boxed{\frac{h}{2} f\left(t_i, w_i\right)}\right)}\right]$$

Recall: RK4 for 1D IVPs

$$w_0 = y(t_0) = \alpha$$

Initial

Step size h

$$k_1 = hf\left(t_{j-1}, w_{j-1}\right)$$

$$k_2 = hf\left(t_{j-1} + \frac{h}{2}, w_{j-1} + \frac{1}{2}k_1\right)$$

$$k_3 = hf\left(t_{j-1} + \frac{h}{2}, w_{j-1} + \frac{1}{2}k_2\right)$$

$$k_4 = hf\left(t_j, w_{j-1} + k_3\right)$$

$$w_j = w_{j-1} + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)$$

$$t_j = t_{j-1} + h$$

Iterative step for t_j (time)

RK4 is typically the best balance between accuracy and cost

RK4 for IVP systems

$$w_{10} = u_1(t_0) = a_1, \quad w_{20} = u_2(t_0) = a_2, \quad \ldots, \quad w_{m0} = u_m(t_0) = a_m$$

Initial

$$k_{1i} = hf_i\left(t_j, w_{1j}, w_{2j}, \ldots w_{mj}\right) \quad \forall i = 1 \ldots m$$

$$k_{2i} = hf_i\left(t_j + \frac{h}{2}, w_{1j} + \frac{k_{11}}{2}, w_{2j} + \frac{k_{12}}{2}, \ldots w_{mj} + \frac{k_{1m}}{2}\right) \quad \forall i = 1 \ldots m$$

$$k_{3i} = hf_i\left(t_j + \frac{h}{2}, w_{1j} + \frac{k_{21}}{2}, w_{2j} + \frac{k_{22}}{2}, \ldots w_{mj} + \frac{k_{2m}}{2}\right) \quad \forall i = 1 \ldots m$$

$$k_{4i} = hf_i\left(t_j + h, w_{1j} + k_{31}, w_{2j} + k_{32}, \ldots w_{mj} + k_{3m}\right) \quad \forall i = 1 \ldots m$$

$$\boxed{w_{i,j+1} = w_{ij} + \frac{1}{6}\left(k_{1i} + 2k_{2i} + 2k_{3i} + k_{4i}\right) \quad \forall i = 1 \ldots m}$$

$$t_{j+1} = t_j + h$$

What is the meaning of i, j, & m?

Example IVP step with RK4

Here is the iterative step that would be used to solve the previous activity's 3D IVP, using RK4 instead of Euler, in terms of w_{ij}, k_{ij}, and h:

$$\boxed{\begin{aligned} w_{1,j+1} &= w_{1j} + \frac{1}{6}\left(k_{11} + 2k_{21} + 2k_{31} + k_{41}\right) \\ w_{2,j+1} &= w_{2j} + \frac{1}{6}\left(k_{12} + 2k_{22} + 2k_{32} + k_{42}\right) \\ w_{3,j+1} &= w_{3j} + \frac{1}{6}\left(k_{13} + 2k_{23} + 2k_{33} + k_{43}\right) \end{aligned}}$$

Example IVP step with RK4

$$k_{11} = hf_1\left(t_j, w_{1j}, w_{2j}, w_{3j}\right) = -2hk_1 w_{1j}^{\;2}$$

$$k_{12} = hf_2\left(t_j, w_{1j}, w_{2j}, w_{3j}\right) = -hk_2 w_{2j} + hk_1 w_{1j}^{\;2}$$

$$k_{13} = hf_3\left(t_j, w_{1j}, w_{2j}, w_{3j}\right) = hk_2 w_{2j}$$

k_1 is the Euler step, as always

$$k_{21} = -2hk_1\left[w_{1j} + \frac{k_{11}}{2}\right]^2$$

$$k_{22} = -hk_2\left[w_{2j} + \frac{k_{12}}{2}\right] + hk_1\left[w_{1j} + \frac{k_{11}}{2}\right]^2$$

$$k_{23} = hk_2\left[w_{2j} + \frac{k_{12}}{2}\right]$$

$$k_{31} = -2hk_1\left[w_{1j} + \frac{k_{21}}{2}\right]^2$$

$$k_{32} = -hk_2\left[w_{2j} + \frac{k_{22}}{2}\right] + hk_1\left[w_{1j} + \frac{k_{21}}{2}\right]^2$$

$$k_{33} = hk_2\left[w_{2j} + \frac{k_{22}}{2}\right]$$

(For more details, see F&B page 215-216)

Example IVP step with RK4

$$k_{41} = -2hk_1\left(w_{1j} + k_{31}\right)^2$$

$$k_{42} = -hk_2\left(w_{2j} + k_{32}\right) + hk_1\left(w_{1j} + k_{31}\right)^2$$

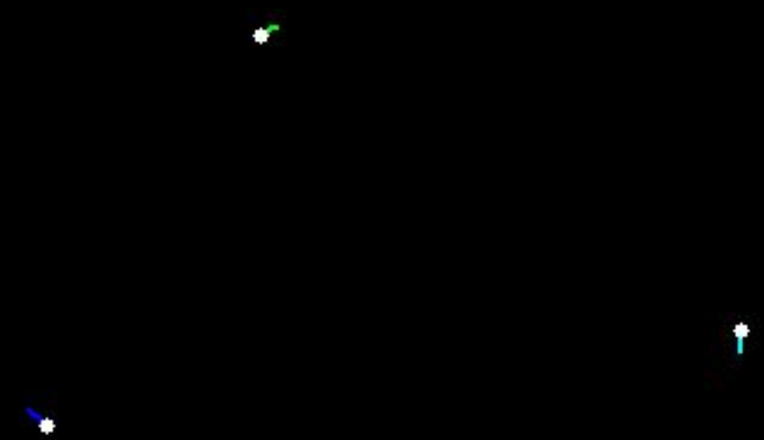
$$k_{43} = hk_2\left(w_{2j} + k_{32}\right)$$

$$\boxed{\begin{aligned} w_{1,j+1} &= w_{1j} + \frac{1}{6}\left(k_{11} + 2k_{21} + 2k_{31} + k_{41}\right) \\ w_{2,j+1} &= w_{2j} + \frac{1}{6}\left(k_{12} + 2k_{22} + 2k_{32} + k_{42}\right) \\ w_{3,j+1} &= w_{3j} + \frac{1}{6}\left(k_{13} + 2k_{23} + 2k_{33} + k_{43}\right) \end{aligned}}$$

$$t_{j+1} = t_j + h$$

Tricky IVPs

Simulation of the 3-body problem (an IVP)



Errors are more likely where the forces are high...

Getting Physics Right

- Low error abs(y_i - y_{true}) is *not* the only goal
- What about conservation laws? Energy, momentum, angular momentum...
- Euler methods, RK4, etc are <u>not energy conserving</u> if used to integrate equations of motion (as in molecular dynamics)
- Energy-conserving methods are called "symplectic" (from the geometry of Hamiltonians, symplectic geometry)

Symplectic Methods

- Most popular: second-order *Velocity Verlet*
- Similar "midpoint" idea to RK2

$$v(t+\frac{1}{2}\Delta t) = v(t) + \frac{1}{2}a(t)\Delta t$$

Estimate the *half-step* velocity, then use it to calculate the whole step

$$x(t+\Delta t) = x(t) + v(t+\frac{1}{2}\Delta t)\Delta t$$

$$a(t+\Delta t) = f(x(t+\Delta t))$$

$$v(t+\Delta t) = v(t+\frac{1}{2}\Delta t) + \frac{1}{2}a(t+\Delta t)\Delta t$$

Symplectic Methods

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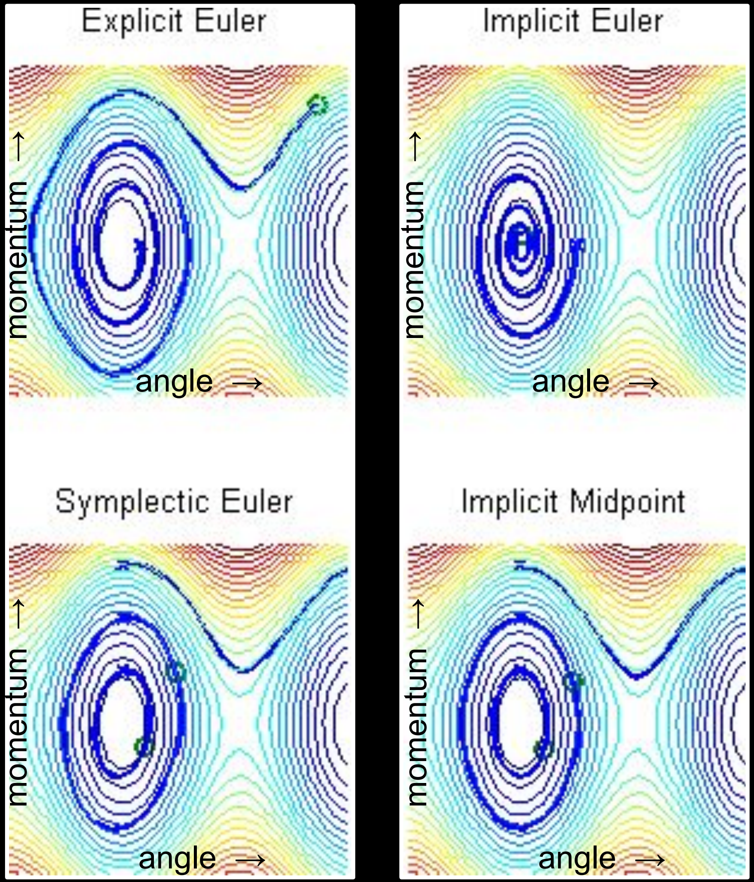

- Dynamics of a frictionless pendulum. Correct solutions are all stable over time (make a ring, not a spiral).
- A method may have low error at every step, like RK45, yet have a steady bias in energy (energy drift) that makes it bad for dynamics simulations

IVPs of a Hamiltonian System

IVPs of a Hamiltonian System