LECTURE 1: Numerical Methods: Integration and ODE&PDEs

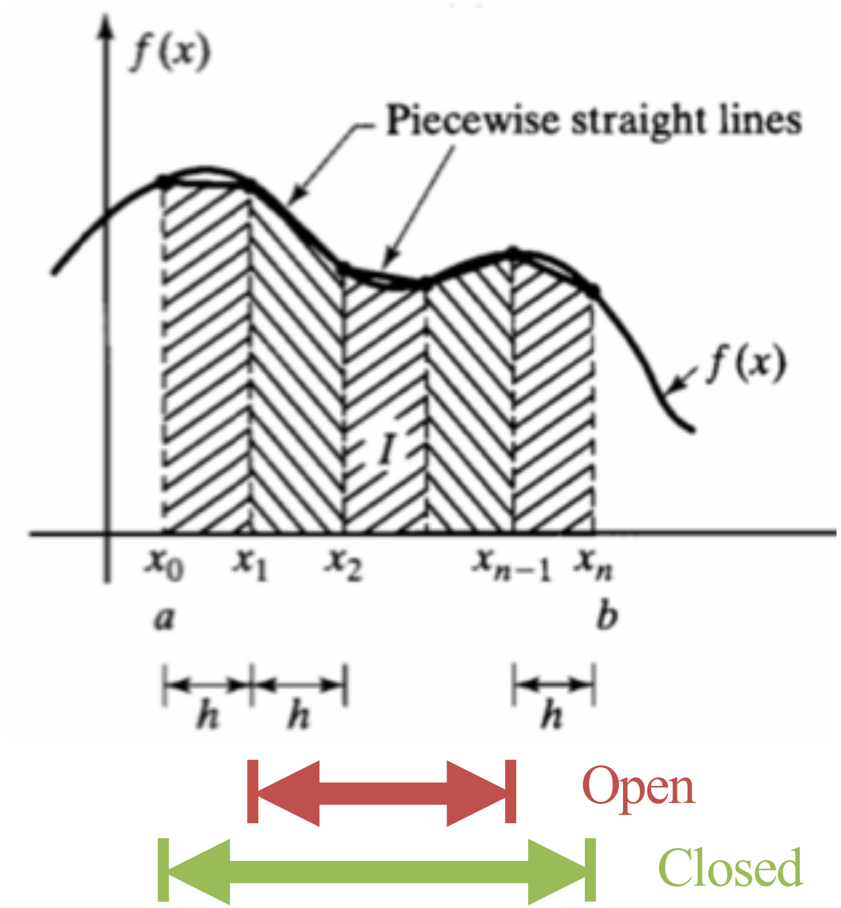
Numerical Integration (also called Quadrature)

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

Special case of differential equation

$$\frac{dy}{dx} = f(x), \; y(a) = 0$$

Simple Trapezoidal Rule



$$x_i = x_0 + ih$$
$$f(x_i) = f_i$$

$$\int_{x_1}^{x_2} f(x)dx =$$
$$\frac{h}{2}(f_1 + f_2) + \mathcal{O}(h^3 f'')$$

- Exact for linear $f(x)$

Image credit: *http://www.unistudyguides.com/wiki/Numerical_Integration*

Simpson's Rule

$$\int_{x_1}^{x_3} f(x)dx = h(\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3) + \mathcal{O}(h^5 f'''')$$

- Exact for $f(x) = \alpha x + \beta x^2 + \gamma x^3$
- Open if we cannot compute $f(x_0)$ or $f(x_{N+1})$

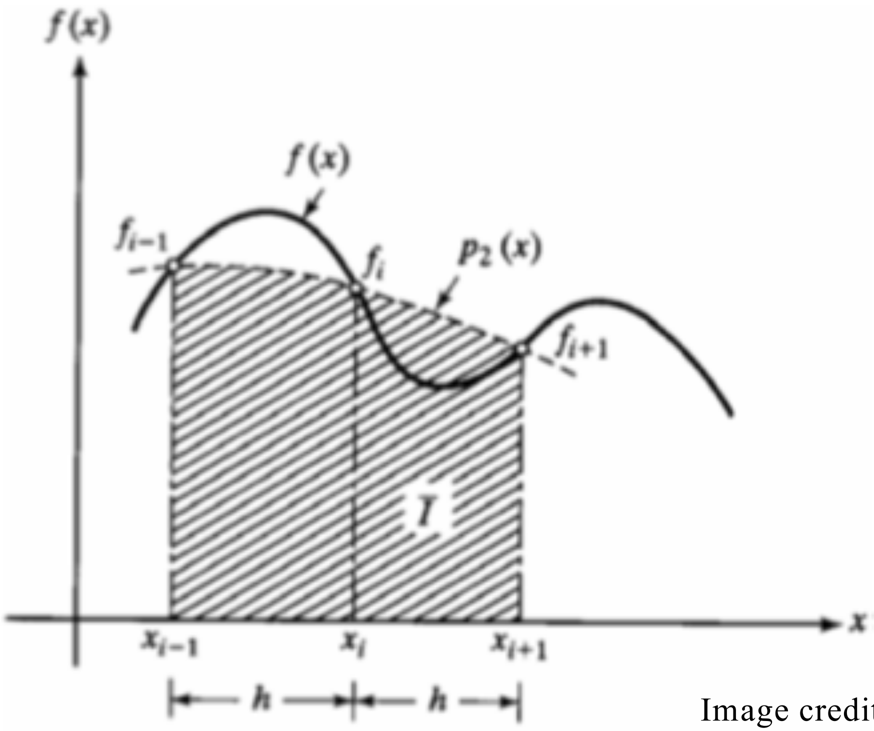


Image credit: *http://www.unistudyguides.com/wiki/Numerical_Integration*

Extended Formula

Trapezoid:
$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{2}f_1 + f_2 + f_3 + \cdots + f_{N-1} + \frac{1}{2}f_N\right] + O\left(\frac{(b-a)^3 f''}{N^2}\right)$$

Simpson:
$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{2}{3}f_3 + \frac{4}{3}f_4 + \cdots + \frac{2}{3}f_{N-2} + \frac{4}{3}f_{N-1} + \frac{1}{3}f_N\right] + O\left(\frac{1}{N^4}\right)$$

Open Extended Trapezoid:
$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{3}{2}f_2 + f_3 + f_4 + \cdots + f_{N-2} + \frac{3}{2}f_{N-1}\right] + O\left(\frac{1}{N^2}\right)$$

- How do we achieve a given accuracy?
- We cannot guess *N* ahead of time, so we need to vary it.

- If we double $N \to 2N$, we can reuse function evaluations.

- Error Estimate: Difference between two subsequent steps
- Also need to put a limit to the number of steps:

$$N_{\max} = 2^{\mathrm{JMAX}-1}, \; \mathrm{JMAX} = 20$$

$\rightarrow$ QTRAP of NR or QSIMP + TRAPZD

- Final refinement: Extended trapezoidal error is even in $1/N$
- *(Euler-MacLaurin summation formula)*:

$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{2}f_1 + f_2 + f_3 + \cdots + f_{N-1} + \frac{1}{2}f_N\right]$$
$$- \frac{B_2 h^2}{2!}(f'_N - f'_1) - \cdots - \frac{B_{2k} h^{2k}}{(2k)!}(f_N^{(2k-1)} - f_1^{(2k-1)}) - \cdots$$

- Apply to N and $2N$: $I = \frac{4}{3}I_{2N} - \frac{1}{3}I_N$ cancels out leading error.

$$I_{\text{true}} = I_N + E_t$$

$$E_t(N) = \frac{C}{N^2} = I_{\text{true}} - I_N \qquad E_t(2N) = \frac{C}{4N^2} = I_{\text{true}} - I_{2N}$$

$$I_{\text{true}} = \frac{4}{3}I_{2N} - \frac{1}{3}I_N$$

$\rightarrow$ We get Simpson's Rule

Romberg Integration

- Use N, $2N$, $4N$, … to cancel out higher orders $O(N^{-2k})$ using polynomial extrapolation: Richardson extrapolation to h=0

Romberg Integration (uses Neville's polynomial interpolation algorithm NR 3.1) → Romberg is the best routine for uniform interval sampling

Doubling N from I_1 to I_2,

$$I_1 + ch_1^2 = I_2 + ch_2^2,$$

$$I_2 - I_1 = ch_1^2 - ch_2^2 = 3ch_2^2,$$

$$\epsilon_2 = ch_2^2 = \tfrac{1}{3}(I_2 - I_1).$$

$$R_{i,1} = I_i\,,$$

$$R_{i,2} = I_i + \tfrac{1}{3}(I_i - I_{i-1}) = R_{i,1} + \tfrac{1}{3}(R_{i,1} - R_{i-1,1}).$$

$$\begin{array}{lllllllll}
I_1 \equiv R_{1,1} & & & & & & & & \\
& \searrow & & & & & & & \\
I_2 \equiv R_{2,1} & \rightarrow & R_{2,2} & & & & & & \\
& \searrow & & \searrow & & & & & \\
I_3 \equiv R_{3,1} & \rightarrow & R_{3,2} & \rightarrow & R_{3,3} & & & & \\
& \searrow & & \searrow & & \searrow & & & \\
I_4 \equiv R_{4,1} & \rightarrow & R_{4,2} & \rightarrow & R_{4,3} & \rightarrow & R_{4,4} & & \\
& \searrow & & \searrow & & \searrow & & \searrow &
\end{array}$$

Improper Integrals

- Cannot be evaluated Ex) $\left.\dfrac{\sin(x)}{x}\right|_{x=0}$

Use open formula: Extended Midpoint Rule

- Infinite boundary Ex) $\displaystyle\int_{-\infty}^{\infty} f(x)dx$
- Integrable singularity Ex) $\displaystyle\int_{0}^{x_0} x^{-\frac{1}{2}}dx$

Change of variables

$$\int_a^b f(x)dx = \int_{1/b}^{1/a} \frac{1}{t^2}\cdot f(1/t)dt$$

$ab > 0$

$b \to \infty, a > 0$

$a \to -\infty, b < 0$

Examples: Change of variables

- Integrable singularity

If the integrand diverges as $(x-a)^{-\gamma}$,
$0 \leq \gamma < 1$, near $x = a$,

$$\int_a^b f(x)dx = \frac{1}{1-\gamma}\int_0^{(b-a)^{1-\gamma}} t^{\frac{\gamma}{1-\gamma}} f(t^{\frac{1}{1-\gamma}} + a)dt \qquad (b > a)$$

- Exponential fall-off

$$t = e^{-x} \qquad \text{or} \qquad x = -\log t$$

$$\int_{x=a}^{x=\infty} f(x)dx = \int_{t=0}^{t=e^{-a}} f(-\log t)\frac{dt}{t}$$

Gaussian Quadratures

- Move beyond equally spaced points
- Choose abscissas and weights, achieving twice the order of accuracy
- Higher order $\neq$ Higher accuracy!
- We can choose to be high accuracy for polynomial times a function *W(x)*

$$\int_a^b W(x) f(x) dx \approx \sum_{j=1}^{N} w_j f(x_j)$$

Weights & Abscissas tabulated for several cases

Read about orthogonal polynomials construction of weights & abscissas in NR

- Commonly used cases:

Rescale for other intervals

Gauss-Legendre:

$$W(x) = 1 \qquad -1 < x < 1$$

Gauss-Chebyshev:

$$W(x) = (1 - x^2)^{-1/2} \qquad -1 < x < 1$$

Gauss-Laguerre:

$$W(x) = x^\alpha e^{-x} \qquad 0 < x < \infty$$

Gauss-Hermite:

$$W(x) = e^{-x^2} \qquad -\infty < x < \infty$$

Gauss-Jacobi:

$$W(x) = (1 - x)^\alpha (1 + x)^\beta \qquad -1 < x < 1$$

Multidimensional Integrals

are HARD!

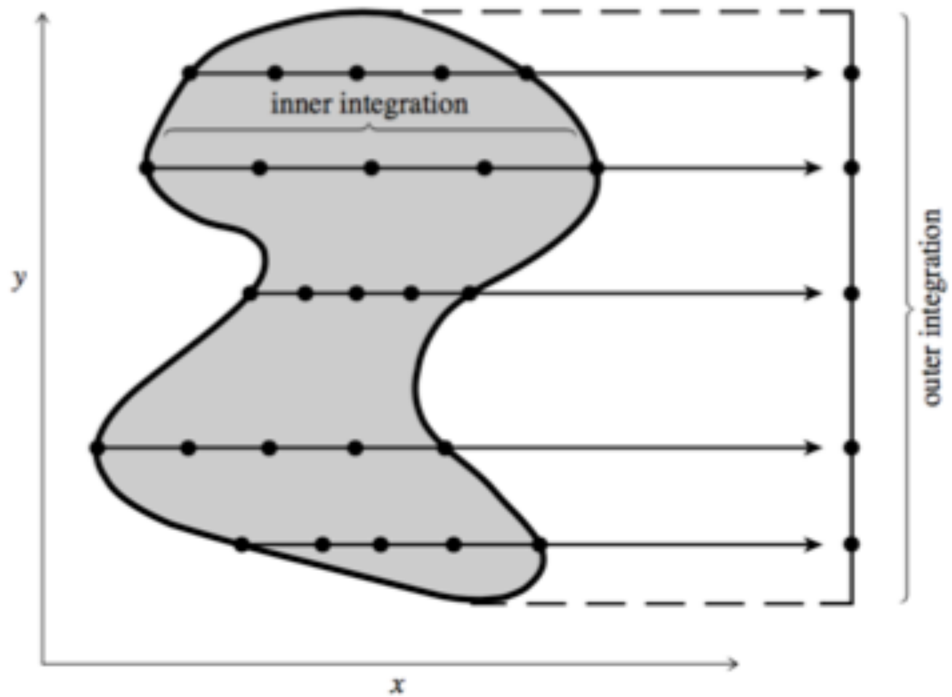
- Number of points scales as N^M, where M: # of dimensions
- Boundary can be complicated

Can dimension be reduced?

$$\int_0^x dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_3} dt_2 \int_0^{t_2} f(t_1) dt_1 = \frac{1}{(n-1)!} \int_0^x (x-t)^{n-1} f(t) dt$$

If complicated boundary, low res, not strongly peaked integrand
$\rightarrow$ Monte Carlo Integration (to be discussed later)

If boundary is simple and function is smooth
$\rightarrow$ Repeated 1-D integrals



$$I = \int\int dx dy f(x,y)$$

$$H(x) = \int_{y_1}^{y_2} f(x,y) dy$$

$$I = \int_{x_1}^{x_2} H(x) dx$$

Best to use Gaussian Quadratures for high precision

Image credit: Press et al., *Numerical Recipes*, 3rd ed. (pg. 198)

Summary

- Workhorse for 1-D integrals is:
  Romberg: simple, nested error estimate

- Input: EPS (Error), Max # of iterations

- If evaluations expensive, use Gaussian Quadratures

- If many dimensions, use 1-D repeated integrals,
  with Gauss Q. preferred

- Complicated boundary + many dim integrals
  → Use Monte Carlo

LECTURE 1: Numerical Methods: Integration and ODE&PDEs

- ODE: in contrast to quadratures there is y dependence f(x,y)
- higher order differential equations can always be rewritten as a series of 1st order:

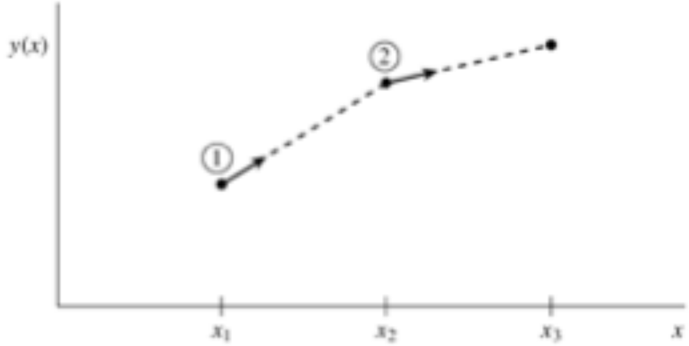
$$\frac{d^2y}{dx^2} + q(x)\frac{dy}{dx} = r(x)$$

$$\frac{dy}{dx} = z(x)$$
$$\frac{dz}{dx} = r(x) - q(x)z(x)$$

- We also need to specify boundary conditions. Typical case is initial value problem: we specify at initial time. For example, specify initial position and velocity of a particle and then use Newton's law to solve for its time evolution

Euler Method, 2nd Order Midpoint …

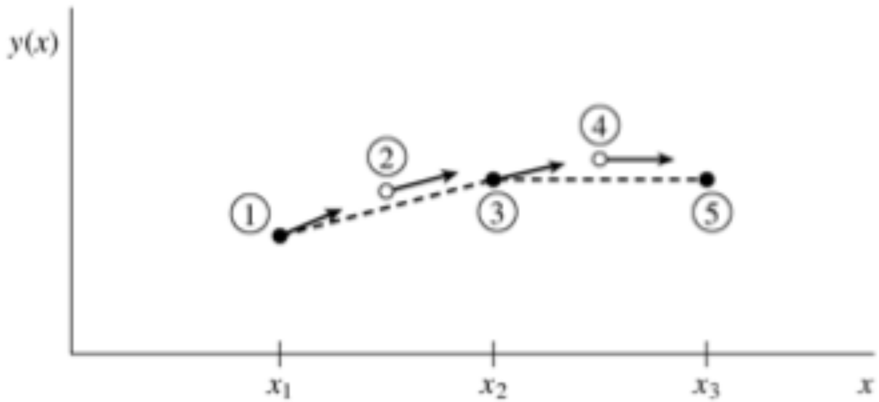
- We start with the simplest method, 1st order (explicit) Euler: *dy/dx = f(x,y), dx = h*



- $$y_{n+1} = y_n + hf(x_n, y_n)$$

- 2nd order extension (midpoint, or 2nd order Runge-Kutta)

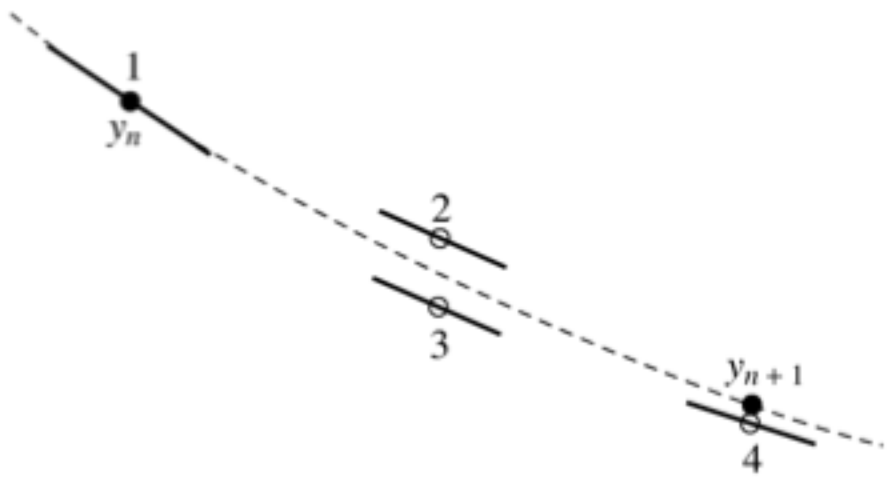
$$k_1 = hf(x_n, y_n)$$
$$k_2 = hf\left(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_1\right)$$
$$y_{n+1} = y_n + k_2 + O(h^3)$$



4th Order Runge-Kutta

- Historically often the method of choice

$$
\begin{aligned}
k_1 &= hf(x_n, y_n) \\
k_2 &= hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_1) \\
k_3 &= hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_2) \\
k_4 &= hf(x_n + h, y_n + k_3) \\
y_{n+1} &= y_n + \tfrac{1}{6}k_1 + \tfrac{1}{3}k_2 + \tfrac{1}{3}k_3 + \tfrac{1}{6}k_4 + O(h^5)
\end{aligned}
$$



4^{th} Order Runge-Kutta

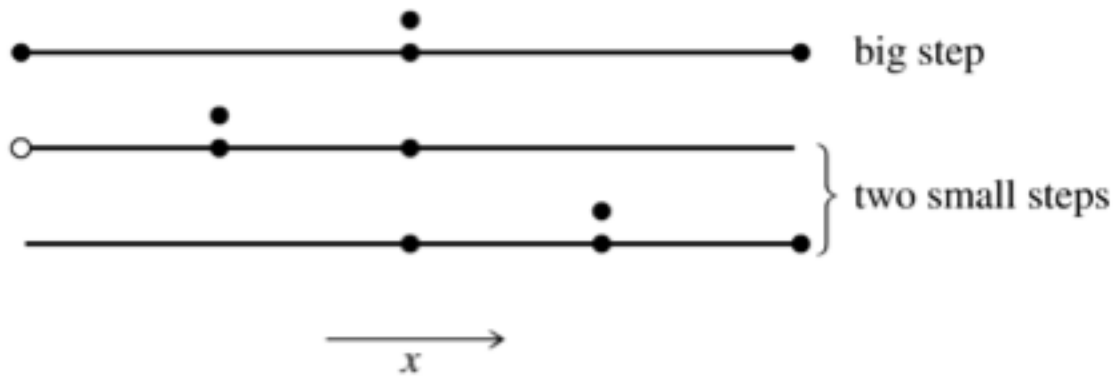
- Add adaptive stepsize control, doubling the step.
- Richardson extrapolation adds one more order

$$y(x+2h) = y_1 + (2h)^5\phi + O(h^6) + \dots$$

$$y(x+2h) = y_2 + 2(h^5)\phi + O(h^6) + \dots$$

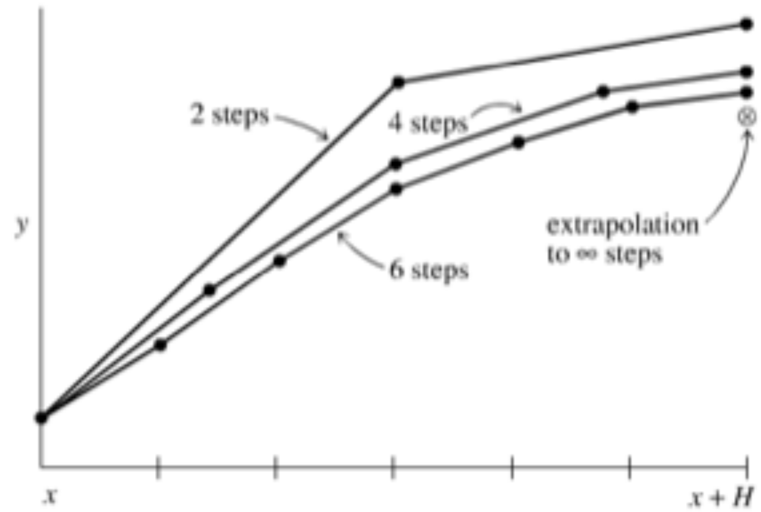
$$y(x+2h) = y_2 + \frac{\Delta}{15} + O(h^6)$$

$$\Delta \equiv y_2 - y_1$$



Bulirsch-Stoer method: "infinite" order extrapolation

- Uses Richardson's extrapolation again (we also used it for Romberg integration): we estimate the error as a function of interval size h, then we try to extrapolate it to h=0
- As in Romberg we need to have the error to be in terms of h^2 powers instead of h
- Can use polynomial or rational function extrapolation: we will discuss both for interpolations

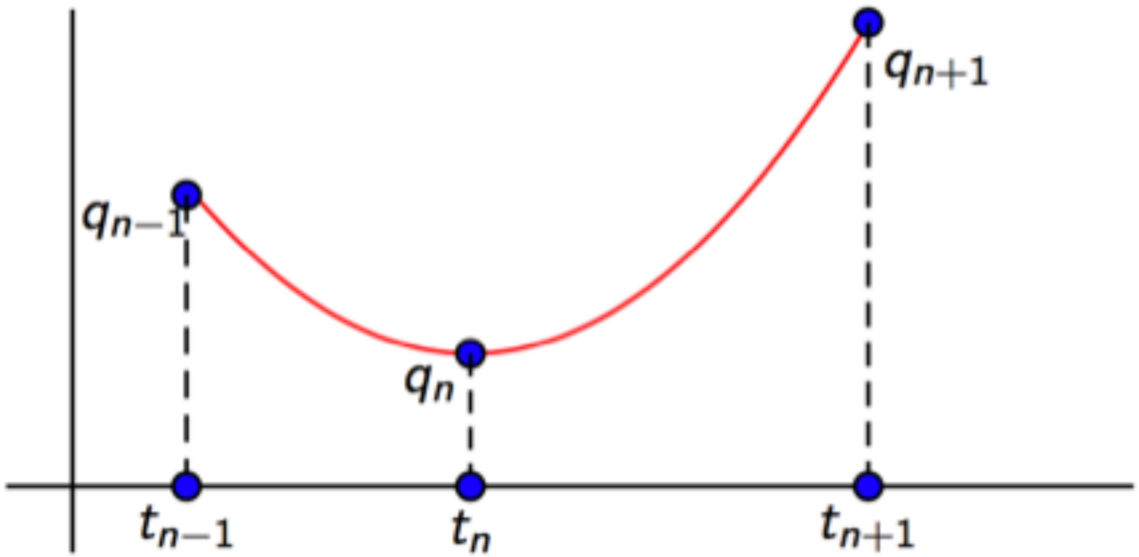


2^{nd} Order Conservative Equations

$$\ddot{q} = f(q)$$

- Stormer-Verlet with two step formulation: we are interpolating parabola through 3 points
- Gains a factor of 2

$$q_{n+1} - 2q_n + q_{n-1} = h^2 f(q_n)$$



One Step Formulation: Leap-frog

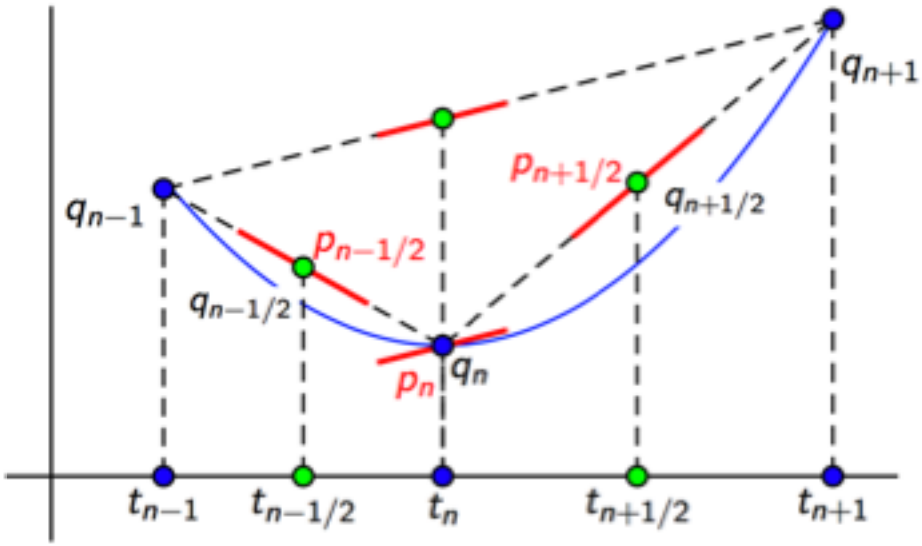
- We introduce momentum $p = \dot{q}, \quad \ddot{q} = f(q)$

$$\dot{q} = p, \qquad \dot{p} = f(q)$$

$$p_{n+1/2} = p_n + \frac{h}{2} f(q_n)$$

$$q_{n+1} = q_n + h p_{n+1/2}$$

$$p_{n+1} = p_{n+1/2} + \frac{h}{2} f(q_{n+1})$$



Generalization: Symplectic Integrators

- Canonical transformation preserves the form of Hamiltonian eq.

Hamilton's equations can be written in a compact form as

$$\dot{z} = J\frac{\partial H}{\partial z}, \tag{33}$$

where $z = (p, q)$ and

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{34}$$

A transformation (mapping) from $z = (p, q)$ to $z' = (p', q')$ can be written as

$$z' = Az, \; A = \frac{\partial z'}{\partial z}, \tag{35}$$

where A is $2x2$ Jacobian transformation matrix.

a) From definitions

$$z' = Az, \; \dot{z} = J\frac{\partial H}{\partial z}, \text{ we have} \tag{44}$$

$$\dot{z}' = A\dot{z} = AJ\frac{\partial H}{\partial z} = AJA^T\frac{\partial H}{\partial z'}. \tag{45}$$

For this to be canonical we need

$$\dot{z}' = J\frac{\partial H}{\partial z'}, \tag{46}$$

hence

$$AJA^T = J. \tag{47}$$

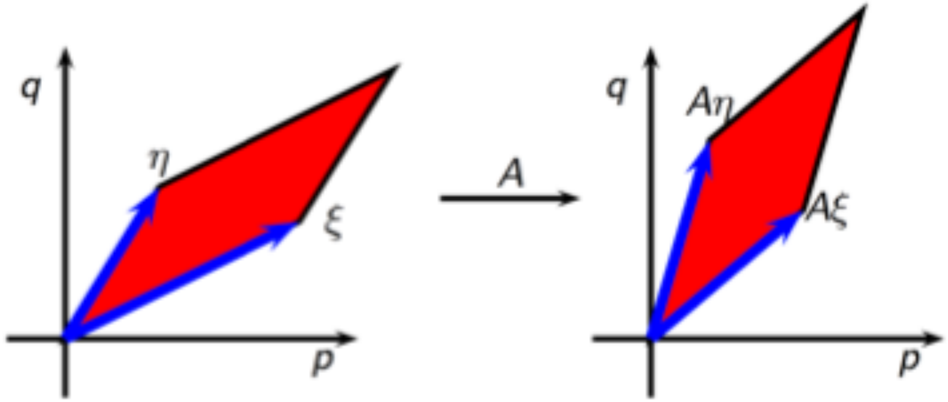
We can also use $z = A^T z'$ and apply the argument in reverse to obtain

$$A^T JA = J. \tag{48}$$

- $A^T JA = AJA^T = J$ iff det $A=1$: this is a symplectic transformation

Generalization: Symplectic Integrators

- Symplectic transformation preserves phase space area (p,q) (Lioville's theorem)



- Proof:

b) Phase space area of a parallelogram S defined by two vectors η and ξ in (p,q) plane can be written in terms of a wedge product as

$$S = \eta^T J \xi. \tag{37}$$

b) We want to determine the area of wedge product $\eta^T J \xi$ under the coordinate transformation $A\eta$ and $A\xi$,

$$S' = (A\eta)^T J(A\xi) = \eta^T A^T J A \xi = \eta^T J \xi, \tag{49}$$

where the last equality follows if A is symplectic, $A^T J A = J$.

Generalization: Symplectic Integrators

- Example: Harmonic oscillator $H(p,q) = \frac{1}{2}\left(p^2 + q^2\right)$

Exact solution of Hamiltonian equations of motion can be viewed as a symplectic transformation from $z = (p, q)$ at time $t = 0$ to $z' = (p', q')$ at $t = \Delta t$. Exact solution can be written as $z' = Az$, with

$$A = \begin{pmatrix} \cos\Delta t & \sin\Delta t \\ -\sin\Delta t & \cos\Delta t \end{pmatrix}. \tag{39}$$

This is a symplectic transformation since $\det A = 1$. The mapping preserves the Hamiltonian, which is conserved (conservation of energy).

A simple first order numerical discretization scheme is Euler's method, which from equation 33 gives,

$$z' = z + \Delta z = z + J\frac{\partial H}{\partial z}\Delta t = \begin{pmatrix} 1 & \Delta t \\ -\Delta t & 1 \end{pmatrix} z. \tag{40}$$

$$\det A = 1 + \Delta t^2 \neq 1, \tag{50}$$

so this transform is not symplectic.

$$H = \frac{1}{2}\left(p'^2 + q'2\right) = \frac{1}{2}\left((q + p\Delta t)^2 + (p - q\Delta t)^2\right) = \frac{1}{2}\left(p^2 + q^2\right)\left(1 + \Delta t^2\right). \tag{51}$$

So energy is not conserved, it increases by $1 + \Delta t^2$ at each integration step. The secular trend is for energy to keep increasing.

- So Euler's method is not symplectic, but can be made symplectic:

$$q' = q + \frac{\partial H}{\partial p}\Delta t,\ p' = p$$
$$q' = q,\ p' = p - \frac{\partial H}{\partial p}\Delta t, \tag{41}$$

are each symplectic. Show that their product is given by

$$z' = \begin{pmatrix} 1 & \Delta t \\ -\Delta t & 1 - \Delta t^2 \end{pmatrix} z, \tag{42}$$

which is also symplectic. This sequence is called symplectic Euler, and

$$A_1 = \begin{pmatrix} 1 & \Delta t \\ 0 & 1 \end{pmatrix}, \tag{52}$$

and

$$A_2 = \begin{pmatrix} 1 & 0 \\ -\Delta t & 1 \end{pmatrix}. \tag{53}$$

They both have $\det A_1 = \det A_2 = 1$, so they are symplectic. Their product is

$$A_2 A_1 = \begin{pmatrix} 1 & 0 \\ -\Delta t & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ -\Delta t & 1 \end{pmatrix} = \begin{pmatrix} 1 & \Delta t \\ -\Delta t & 1 - \Delta t^2 \end{pmatrix}. \tag{54}$$

Generalization: Symplectic Integrators

- Hamiltonian is not conserved, but a related quantity is and one does not accumulate amplitude error, only phase error

$$
\begin{aligned}
\tilde{H} &= \frac{1}{2}\left(p'^2 + q'2 + \Delta t p' q'\right) \\
&= \frac{1}{2}\left((q + p\Delta t)^2 + (p - q\Delta t)^2 + \Delta t (q + p\Delta t)(p - q\Delta t)\right) \\
&= \frac{1}{2}\left(p^2 + q^2 + \Delta t pq\right), \qquad (55)
\end{aligned}
$$

so $\tilde{H}$ is conserved.

$$\tilde{H} = \frac{1}{2}\left(p^2 + q^2 + pq\Delta t\right), \qquad (43)$$

for a fixed initial value of Δt. Equation 43 describes an ellipse in (p, q) plane, so by repeated mappings of equation 42 the points will lie on an ellipse that differs from the true solution (circle of equation 38) by a term of order Δt. This term cannot grow after repeated mappings, and there is no secular (long term) energy error accumulation for symplectic mappings.

- Symplectic integration is useful if one needs to integrate a system for a long time (e.g. planet orbits etc)

Leapfrog is Symplectic

Hamiltonian problem $\dot{p} = -H_q(p,q)$, $\dot{q} = H_p(p,q)$

Theorem. The Störmer-Verlet method

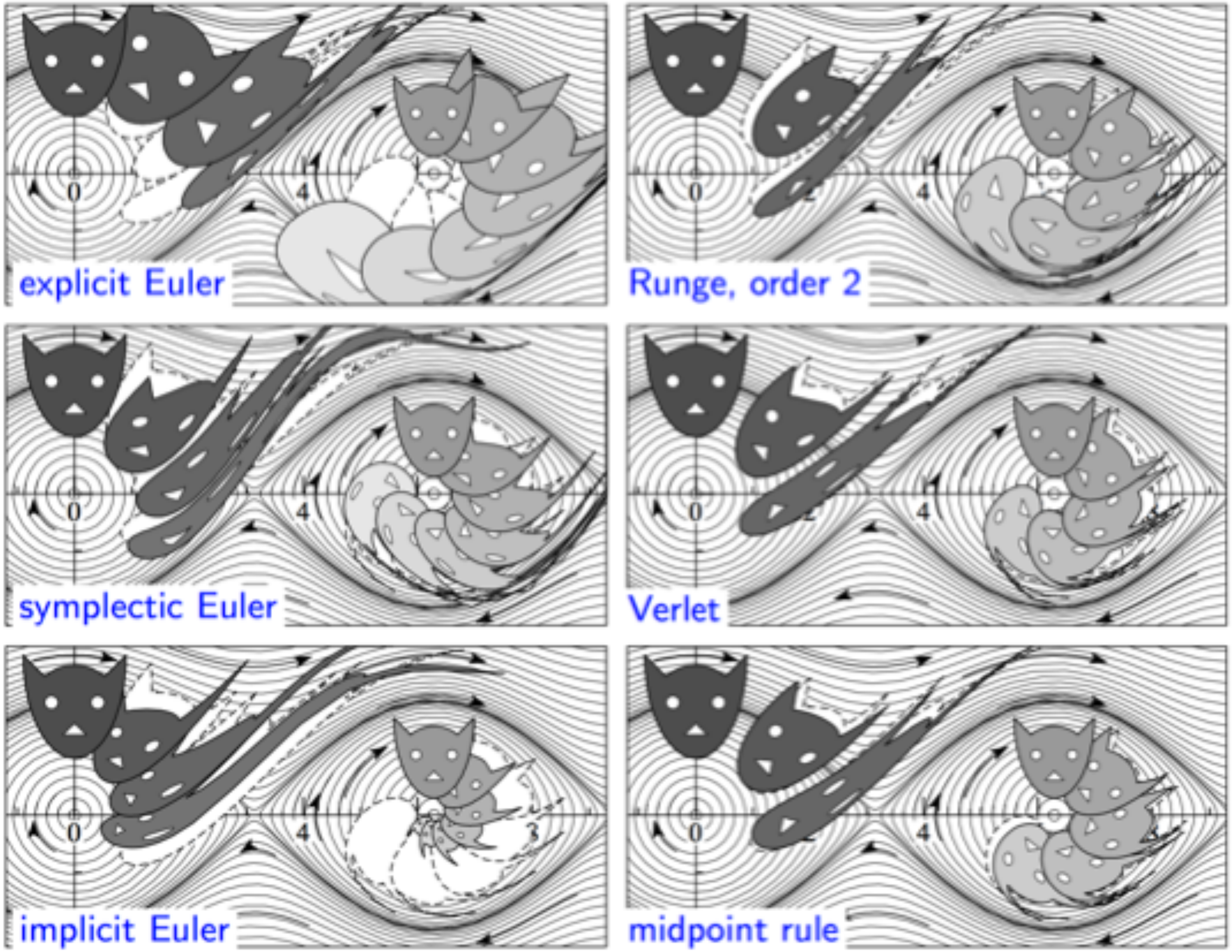
$$p_{n+1/2} = p_n - \frac{h}{2} H_q(p_{n+1/2}, q_n)$$

$$q_{n+1} = q_n + \frac{h}{2}\Big(H_p(p_{n+1/2}, q_n) + H_p(p_{n+1/2}, q_{n+1})\Big)$$

$$p_{n+1} = p_{n+1/2} - \frac{h}{2} H_q(p_{n+1/2}, q_{n+1})$$

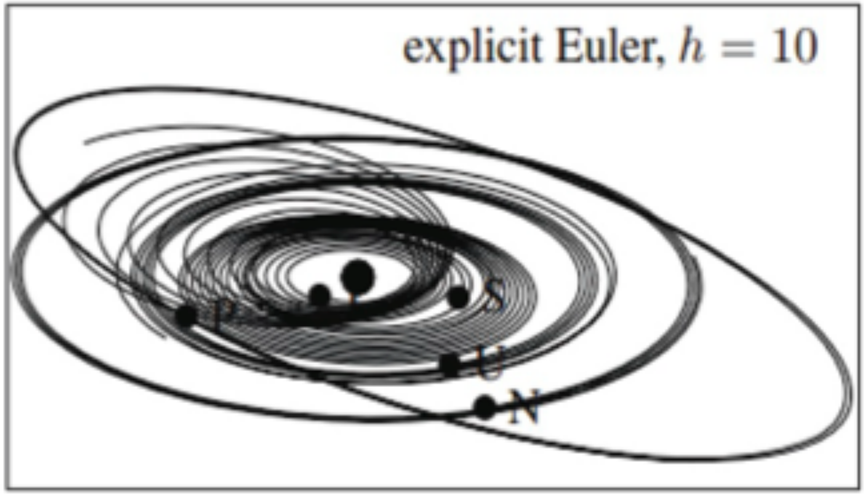
is symplectic.

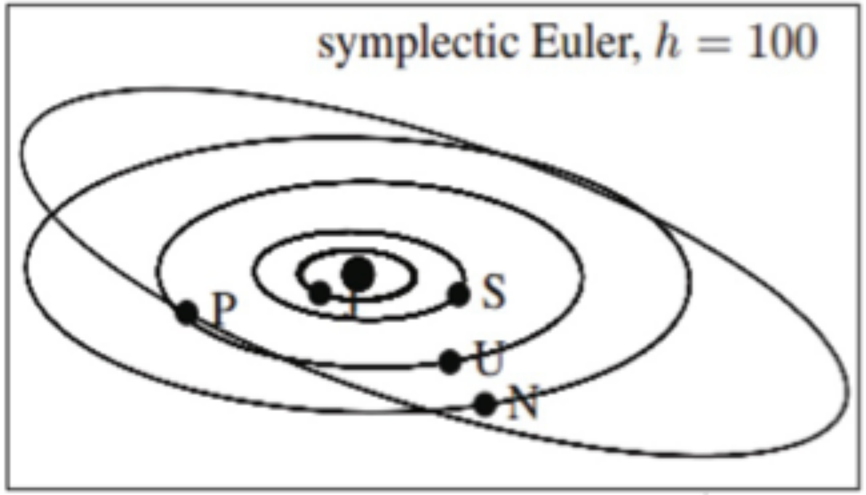
Phase Space Flow



Example: Planetary Orbit Integration

- Explicit Euler's orbits decay. This is not cured by higher order (Runge-Kutta, B-S…)
- Symplectic integrators preserve the orbit amplitude (but not the phases, not shown)





Stiff Equations

- Explicit (forward) Euler:

$$y' = -cy$$

$$y_{n+1} = y_n + hy'_n = (1 - ch)y_n$$

- Unstable if $h > 2/c$, since y goes to infinity
- Example:

$$u' = 998u + 1998v \qquad u(0) = 1 \qquad v(0) = 0$$

$$v' = -999u - 1999v$$

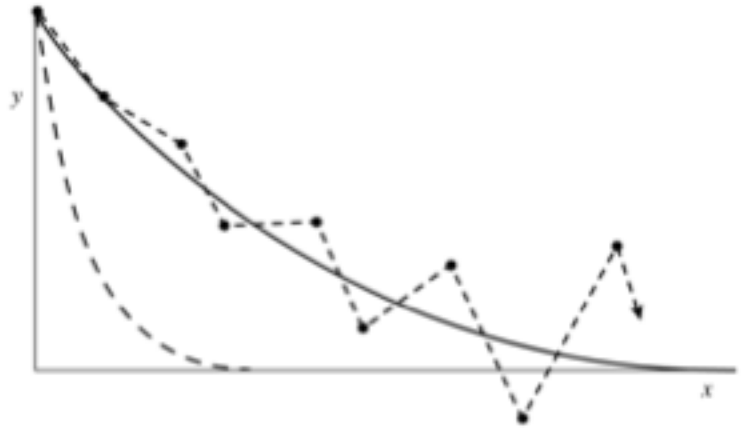
$$u = 2e^{-x} - e^{-1000x}$$

$$u = 2y - z \qquad v = -y + z \qquad v = -e^{-x} + e^{-1000x}$$

- But the system is unstable if h > 1/1000
- Solution: implicit (backward Euler)

$$y_{n+1} = y_n + hy'_{n+1}$$

$$y_{n+1} = \frac{y_n}{1 + ch}$$



General Approach

- If we are solving a linear system: $\mathbf{y}' = -\mathbf{C} \cdot \mathbf{y}$

$$\mathbf{T}^{-1} \cdot \mathbf{C} \cdot \mathbf{T} = \mathrm{diag}(\lambda_0 \dots \lambda_{N-1}) \qquad \mathbf{z}' = -\mathrm{diag}(\lambda_0 \dots \lambda_{N-1}) \cdot \mathbf{z}$$

$$\mathbf{z} = \mathrm{diag}(e^{-\lambda_0 x} \dots e^{-\lambda_{N-1} x}) \cdot \mathbf{z}_0$$

- Exact solution: $\mathbf{y} = \mathbf{T} \cdot \mathrm{diag}(e^{-\lambda_0 x} \dots e^{-\lambda_{N-1} x}) \cdot \mathbf{T}^{-1} \cdot \mathbf{y}_0$

- Explicit scheme: $\mathbf{y}_0 = \sum_{i=0}^{N-1} \alpha_i \boldsymbol{\xi}_i \qquad \mathbf{y}_n = \sum_{i=0}^{N-1} \alpha_i (1 - h\lambda_i)^n \boldsymbol{\xi}_i$

- Stability condition: $|1 - h\lambda_i| < 1 \qquad i = 0, \dots, N-1 \qquad h < \frac{2}{\lambda_{\max}}$

- Implicit scheme: $\mathbf{y}_{n+1} = (\mathbf{1} + \mathbf{C}h)^{-1} \cdot \mathbf{y}_n$

- Always stable: $|1 + h\lambda_i|^{-1} < 1 \qquad i = 0, \dots, N-1$

Stiff Nonlinear Equations

- In general, implicit scheme hard to solve

$$\mathbf{y}' = \mathbf{f}(\mathbf{y})$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(\mathbf{y}_{n+1})$$

- Linearize f : (Newton's method)

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\left[\mathbf{f}(\mathbf{y}_n) + \left.\frac{\partial \mathbf{f}}{\partial \mathbf{y}}\right|_{\mathbf{y}_n} \cdot (\mathbf{y}_{n+1} - \mathbf{y}_n)\right]$$

- Invert Jacobian:

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\left[\mathbf{1} - h\frac{\partial \mathbf{f}}{\partial \mathbf{y}}\right]^{-1} \cdot \mathbf{f}(\mathbf{y}_n)$$

- This is semi-implicit Euler method
- There are also stiff versions of higher order ODE

Partial Differential Equations

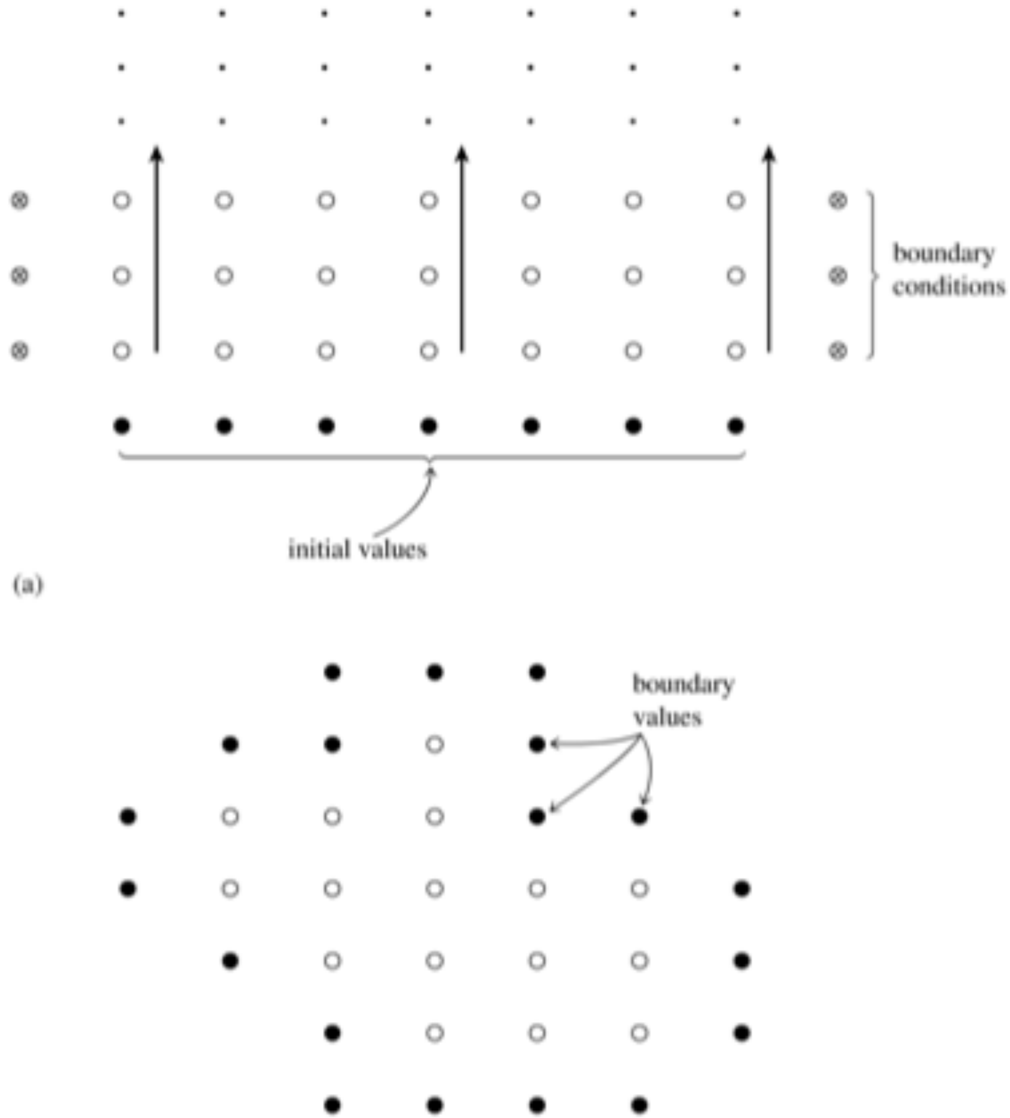
- This is a vast subject, and we will only mention its existence
- Hyperbolic, e.g. wave equation: $\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$
- Parabolic, e.g. diffusion equation: $\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial u}{\partial x}\right)$
- Both of these are initial value (Cauchy) problems
- Boundary value problem: elliptic, Elliptic, e.g. Poisson equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x, y)$$

- If source ρ=0 this is Laplace equation

Finite Difference Method

- Discretize on a grid…



Summary

- ODEs and PDEs are central to numerical analysis in physical sciences, engineering…
- ODEs have a relatively stable methods
- PDEs have a vast array of approaches: relaxation, finite differences, finite elements, spectral methods, matrix methods, multi-grid, Monte Carlo, variational…

Literature

Numerical Integration:

- *Numerical Recipes*, Press et al., Chapter 4
  (http://apps.nrbook.com/c/index.html)
- *Computational Physics*, Mark Newman, Chapter 5
  (http://www-personal.umich.edu/~mejn/cp/chapters/int.pdf)

ODE&PDEs

- *Numerical Recipes*, Press et al., Chapter 17-20