

TAOCP Vol. 2 + Numerical Recipes

Numerical Calculus Study Deck

Kanban-oriented StoryCards grouped by Phases

Kanban Board Overview

Kanban Columns & Tags

Board Columns:

- **Backlog** – All reading and implementation cards not yet started.
- **In Progress** – Cards currently being read, coded, or experimented on.
- **Review / Experiments** – Numerical experiments, derivations, error analysis, refactors.
- **Done / Consolidated** – Code implemented, tested, documented, and integrated into the library.

Recommended Tags (examples):

- **Book tags:** Book:TAOCP2, Book:NR.
- **Module tags:** Module:core-fp, Module:core-poly, Module:interp, Module:quad, Module:ode, Module:nonlin, Module:linalg, Module:rand, Module:optim, Module:stats.
- **Work type tags:** Reading, Implementation, Experiment, Design, Refactor.

Usage Pattern:

- Each *StoryCard* in this document corresponds to a Kanban card.
- Start with Phase 0 cards in *Backlog*. Pull into *In Progress* with a strict WIP limit (e.g., max 2–3 cards).
- Move to *Review / Experiments* once code compiles and basic tests run.
- Move to *Done / Consolidated* only when:
 - There is at least one unit test or numerical experiment.
 - The API is sketched and documented in the repo.
 - You have brief notes in your study log.

Phase 0 – Environment & Test Harness

Phase 0 Overview – Environment & Test Harness

Goal: Be able to quickly prototype, run, and visualize numerical methods from TAOCP Vol. 2 and Numerical Recipes.

Primary Focus:

- Project layout and build system.
- Test harness and plotting workflow.
- Basic utilities for timing and error measurement.

Module Tie-ins:

- `Module:all` (infrastructure for every module).

Exit Criteria:

- You can write a small numerical routine, compile it, run it, compute error metrics, and plot the results with minimal friction.
- The repo layout is stable enough that later phases only add modules, not re-architect the whole tree.

Phase 0 Card 1 – Set Up Numerical Playground Repo

Description: Create a dedicated repository to host your computational math system and numerical experiments.

Checklist:

- ☐ Create a root layout such as:
 - `core/` (floating point, utilities, polynomials).
 - `interp/` (interpolation and approximation).
 - `integrate/` (quadrature / integration).
 - `ode/` (ordinary differential equations).
 - `opt/` (optimization).
 - `rand/` (random numbers and Monte Carlo).
 - `nonlin/` (root finding and nonlinear systems).
 - `linalg/` (linear algebra).
 - `stats/` (error/statistics tools).
 - `examples/`, `tests/`, `docs/`.
- ☐ Add a basic C/C++ build system:
 - `CMakeLists.txt` or equivalent build file.
 - Configurable build type (Debug/Release).
- ☐ Integrate a simple test harness:
 - Minimal custom test main, or
 - Catch2 / GoogleTest wired into the build.
- ☐ Add a plotting hook:
 - Helper to dump (`x`, `y`) data to CSV.
 - Document how to plot via Python/Matplotlib or gnuplot.

Deliverables:

- Repository skeleton committed (e.g., Git).
- `README.md` describing layout, build, and plotting workflow.

Tags: `Infra`, `Module:all`, `Implementation`

Phase 0 Card 2 – Implement Timing & Error Metrics Utilities

Description: Provide reusable helpers for timing functions and computing numerical error metrics.

Checklist:

- ☐ Implement timing helpers:
 - Wall-clock timer based on `std::chrono` (or platform equivalent).
 - Scope-based timer to measure function runtimes.
- ☐ Implement error metric utilities:
 - Absolute error: $|x - x_{\text{true}}|$.
 - Relative error: $\frac{|x - x_{\text{true}}|}{|x_{\text{true}}|}$.
 - Max norm over a dataset.
 - RMS error over samples.
- ☐ Implement convergence-rate estimator:
 - Given error values for step sizes $h, h/2, h/4$, estimate observed order p .
- ☐ Add minimal tests:
 - Check that zero error is reported correctly.
 - Check that known error cases behave as expected.

Deliverables:

- `core/timing.h`, `core/timing.cpp`.
- `core/error_metrics.h`, `core/error_metrics.cpp`.
- A small example program demonstrating timing and error calculations.

Tags: `Module:core-fp`, `Implementation`, `Experiment`

Phase 1 – Core Arithmetic, Error & Representation

Phase 1 Overview – Core Arithmetic, Error & Representation

Goal: Understand how the machine represents numbers and how that shapes numerical error in calculus algorithms.

Primary Sources:

- TAOCP Vol. 2, Chapter 4: arithmetic, floating-point, polynomial and power-series arithmetic.
- Numerical Recipes:
 - Chapter 1: error, accuracy, stability.
 - Chapter 5: evaluation of functions (polynomials, series).

Module Tie-ins:

- `core::fp` (floating-point utilities).
- `core::poly` (polynomial arithmetic and evaluation).

Exit Criteria:

- You can quantify and visualize rounding error and cancellation.
- You have a robust implementation of polynomial evaluation (Horner) with tests.

Phase 1 Card 1 – Read Floating-Point Arithmetic & Rounding

Description: Build theoretical understanding of floating-point representation, rounding, and error propagation.

Reading Tasks:

- TAOCP Vol. 2, sections 4.1–4.2:
 - Positional number systems.
 - Floating-point formats and rounding modes.
- Numerical Recipes, Section 1.1:
 - Error, accuracy, and stability.
 - Conditioning vs. algorithmic stability.

Notes Deliverable:

- A one-page summary covering:
 - Definition of machine epsilon for your platform.
 - Examples of catastrophic cancellation.
 - Distinction between well-conditioned problems and stable algorithms.

Tags: Reading, Book:TAOCP2, Book:NR, Module:core-fp

Phase 1 Card 2 – Implement Safe Floating-Point Utilities

Description: Translate the theory into a `core::fp` utility module.

Checklist:

- ☐ Implement `double ulp(double x)`:
 - Approximate the distance between representable numbers around `x`.
- ☐ Implement `bool nearly_equal(double a, double b)`:
 - Combine absolute and relative tolerance.
- ☐ Implement robust summation:
 - Naive summation for baseline.
 - Kahan summation or pairwise summation.
- ☐ Add tests:
 - Show difference between naive and Kahan for ill-conditioned sums.
 - Verify that `nearly_equal` behaves correctly for small and large magnitudes.

Deliverables:

- `core/fp.h`, `core/fp.cpp`.
- A small example that sums a sequence known to illustrate cancellation, with printed error statistics.

Tags: `Module:core-fp`, `Implementation`, `Experiment`

Phase 1 Card 3 – Read & Implement Polynomial Evaluation

Description: Use TAOCP and NR to implement efficient polynomial evaluation and test its numerical behavior.

Reading Tasks:

- ☐ TAOCP Vol. 2, section 4.6 (polynomial arithmetic, Horner's rule).
- ☐ Numerical Recipes, section 5.1 (polynomials and rational functions).

Implementation Tasks:

- ☐ Design a polynomial representation:
 - Coefficient array in ascending order (constant term first).
 - Or a small `Poly` class with degree and coefficients.
- ☐ Implement `poly_eval` using Horner's rule.
- ☐ Optionally implement polynomial addition and multiplication (for later Chebyshev work).

Experiment Tasks:

- ☐ Choose test polynomials (e.g., Chebyshev, Taylor expansions).
- ☐ Evaluate them at many points and compare:
 - Direct evaluation vs. Horner's rule.
 - Error vs. degree when approximating known functions.

Deliverables:

- `core/poly.h`, `core/poly.cpp`.
- Plots or tables of error vs. degree for at least one approximation problem.

Tags: `Module:core-poly`, Reading, Implementation, Experiment

Phase 2 – Interpolation & Approximation

Phase 2 Overview – Interpolation & Approximation

Goal: Build interpolation and approximation tools that will feed into differentiation, integration, and ODE/PDE solvers.

Primary Sources:

- TAOCP Vol. 2, sections 4.6 and 4.7 (polynomials and power series).
- Numerical Recipes, Chapter 3 (interpolation and extrapolation), and sections 5.8–5.10 (Chebyshev approximation).

Module Tie-ins:

- `interp::` (interpolation).
- `core::poly` (polynomial arithmetic).

Exit Criteria:

- You can construct interpolation schemes and Chebyshev approximations.
- You can compare errors for different node distributions and degrees.

Phase 2 Card 1 – Read Interpolation Basics

Description: Understand the basic interpolation methods and their properties.

Reading Tasks:

- ☐ Numerical Recipes, Chapter 3, sections 3.0–3.3:
 - Table lookup, polynomial interpolation, cubic splines.
- ☐ Skim sections on multidimensional interpolation (3.6–3.7) for later.

Notes Deliverable:

- Short notes summarizing:
 - When polynomial interpolation is appropriate.
 - Why splines can be more stable.
 - Dangers of extrapolation.

Tags: Reading, Book:NR, Module:interp

Phase 2 Card 2 – Implement 1D Interpolation Module

Description: Implement core 1D interpolation routines.

Implementation Tasks:

- ☐ Implement polynomial interpolation:
 - Given arrays `x[i]`, `y[i]`, construct coefficients or direct evaluation routines.
- ☐ Implement cubic splines:
 - Natural or clamped boundary conditions.
 - Precompute spline coefficients; expose an evaluation function.
- ☐ Design a clean API:
 - `interp::poly(x, y)` returning an object with an `operator()`.
 - `interp::spline(x, y)` similarly.

Testing & Experiments:

- ☐ Test on smooth functions (e.g., $\sin x$, $\exp x$) and less smooth ones.
- ☐ Compare interpolation error for different numbers of nodes.

Deliverables:

- `interp/interp.h`, `interp/interp.cpp`.
- Example program visualizing interpolated curves vs. ground truth.

Tags: `Module:interp`, `Implementation`, `Experiment`

Phase 2 Card 3 – Implement Chebyshev Approximation

Description: Implement Chebyshev-based function approximation and connect it to polynomial arithmetic.

Reading Tasks:

- ☐ Numerical Recipes, sections 5.8–5.10:
 - Chebyshev approximation, derivatives, and integrals via coefficients.
- ☐ Revisit TAOCP Vol. 2, section 4.6 for efficient polynomial evaluation and composition.

Implementation Tasks:

- ☐ Implement routines to compute Chebyshev coefficients of a function on $[-1, 1]$.
- ☐ Implement evaluation of the Chebyshev approximation at arbitrary points.
- ☐ Provide helpers to differentiate/integrate the Chebyshev approximation.

Experiment Tasks:

- ☐ Approximate several functions (e.g., $\sin x$, $\exp x$, a Gaussian).
- ☐ Compare approximation error vs. degree for Chebyshev vs. naive polynomial interpolation.

Deliverables:

- `interp/chebyshev.h`, `interp/chebyshev.cpp`.
- Plots of error vs. polynomial degree and node distributions.

Tags: `Module:interp`, `Module:core-poly`, `Implementation`, `Experiment`

Phase 2 Card 4 – Experiment: Interpolation vs Degree & Nodes

Description: Dedicated experiments on the behavior of interpolation as degree and node distribution change.

Experiment Tasks:

- ☐ Choose several test functions:
 - Smooth ($\sin x$, $\exp x$).
 - With endpoint features or mild singularities.
- ☐ Compare:
 - Equally spaced nodes vs. Chebyshev nodes.
 - Polynomial interpolation vs. splines vs. Chebyshev approximation.
- ☐ Produce plots of:
 - Max error vs. degree.
 - Error distribution across the interval.

Deliverables:

- An `examples/interp_study.cpp` (or similar) program.
- A short write-up summarizing observations (Runge phenomenon, stability).

Tags: `Module:interp`, `Experiment`, `Analysis`

Phase 3 – Numerical Differentiation & Integration (Quadrature)

Phase 3 Overview – Numerical Differentiation & Integration

Goal: Directly attack core calculus tasks: derivative estimation and definite integrals.

Primary Sources:

- Numerical Recipes:
 - Section 5.7: numerical derivatives and error behavior.
 - Chapter 4: integration of functions (classical formulas, Romberg, Gaussian, adaptive, multidimensional).

Module Tie-ins:

- `diffint::deriv` (differentiation).
- `diffint::quad` (quadrature).

Exit Criteria:

- You have derivative estimators and quadrature routines with observed convergence rates matching theory.
- You can visualize error vs. step size or number of function evaluations.

Phase 3 Card 1 – Read Numerical Differentiation & Error Behavior

Description: Build conceptual understanding of finite differences and their errors.

Reading Tasks:

- Numerical Recipes, section 5.7:
 - Forward, backward, and central differences.
 - Step-size tradeoffs between truncation and round-off error.

Notes Deliverable:

- Short notes or a diagram showing:
 - Taylor-expansion-based derivation of finite-difference formulas.
 - Qualitative shape of error vs. step size (U-shaped curve).

Tags: Reading, Book:NR, Module:diffint-deriv

Phase 3 Card 2 – Implement Derivative Estimators

Description: Implement a small `diffint::deriv` module.

Implementation Tasks:

- ☐ Implement:
 - `deriv_forward(f, x, h).`
 - `deriv_backward(f, x, h).`
 - `deriv_central(f, x, h).`
- ☐ Optionally add Richardson extrapolation to boost accuracy.
- ☐ Use `core::fp` utilities for error comparisons.

Experiment Tasks:

- ☐ For known functions (e.g., $\sin x$, $\exp x$, polynomials):
 - Sweep over step sizes h .
 - Plot absolute error vs. h for each scheme.
 - Show the “sweet spot” where truncation and round-off balance.

Deliverables:

- `diffint/deriv.h`, `diffint/deriv.cpp`.
- Example program producing error plots.

Tags: `Module:diffint-deriv`, `Implementation`, `Experiment`

Phase 3 Card 3 – Read Integration Methods Overview

Description: Survey classical quadrature methods.

Reading Tasks:

- Numerical Recipes, sections 4.0–4.4:
 - Trapezoidal rule, Simpson’s rule, Romberg integration.
 - Basics of improper integrals.

Notes Deliverable:

- A small table summarizing:
 - Order of accuracy for each rule.
 - When each method is appropriate or problematic.

Tags: Reading, Book:NR, Module:diffint-quad

Phase 3 Card 4 – Implement Basic 1D Quadrature

Description: Implement basic 1D integration routines.

Implementation Tasks:

- ☐ Implement composite trapezoidal rule: `trap(f, a, b, n)`.
- ☐ Implement composite Simpson's rule: `simpson(f, a, b, n)`.
- ☐ Implement Romberg integration `romberg(f, a, b)` using trapezoidal estimates.

Experiment Tasks:

- ☐ Integrate known functions (polynomials, $\sin x$, $\exp x$):
 - Compare numerical results to analytic integrals.
 - Plot error vs. number of function evaluations.

Deliverables:

- `diffint/quad.h`, `diffint/quad.cpp`.
- Example program for integration convergence plots.

Tags: `Module:diffint-quad`, `Implementation`, `Experiment`

Phase 3 Card 5 – Implement Advanced Quadrature & Convergence Plots

Description: Extend the integration module with more advanced schemes and compare their performance.

Implementation Tasks:

- ☐ Implement Gaussian quadrature:
 - `gauss_legendre(f, a, b, n)`.
- ☐ Implement an adaptive integrator:
 - Subdivide intervals based on local error estimates.
- ☐ Optionally add multidimensional integration wrappers (tensor product or simple Monte Carlo).

Experiment Tasks:

- ☐ For several test integrals:
 - Compare error vs. function evaluations for trapezoid, Simpson, Romberg, Gaussian, and adaptive methods.
 - Summarize which method wins for which class of functions.

Deliverables:

- Extended `diffint/quad.*` with advanced methods.
- Plots or tables of convergence behavior.

Tags: `Module:diffint-quad`, Implementation, Experiment, Analysis

Phase 4 – Root Finding & Nonlinear Equations

Phase 4 Overview – Root Finding & Nonlinear Equations

Goal: Solve $f(x) = 0$ and small nonlinear systems using robust algorithms.

Primary Sources:

- Numerical Recipes, Chapter 9:
 - Bracketing methods, secant, Brent, Newton, and nonlinear systems.

Module Tie-ins:

- `nonlin::root` (root finding).
- `linalg::` (linear algebra for systems).
- `diffint::deriv` (for Newton's method derivatives).

Exit Criteria:

- You have a generic 1D root-finding API with multiple methods.
- You can solve small nonlinear systems using a Newton-style method.

Phase 4 Card 1 – Read Root-Finding Landscape

Description: Understand the tradeoffs between different root-finding methods.

Reading Tasks:

- Numerical Recipes, sections 9.0–9.4:
 - Bracketing methods (bisection).
 - Secant and Brent methods.
 - Newton’s method and its convergence properties.

Notes Deliverable:

- A small table summarizing:
 - Method type (bracketing vs. open).
 - Convergence rate.
 - Requirements (derivative? initial bracket?).

Tags: Reading, Book:NR, Module:nonlin-root

Phase 4 Card 2 – Implement 1D Root-Finding API

Description: Implement a small `nonlin::root` module with multiple strategies.

Implementation Tasks:

- ☐ Implement:
 - `bisect(f, a, b, tol)`.
 - `newton(f, df, x0, tol)`.
 - `brent(f, a, b, tol)`.
- ☐ Provide a unified wrapper:
 - `root_find(f, ...)` that selects method based on configuration.
- ☐ Use finite differences from `diffint::deriv` when analytic derivatives are not available.

Experiment Tasks:

- ☐ Test on several functions with known roots:
 - Polynomials of moderate degree.
 - Transcendental equations ($\sin x = x/2$, etc.).
- ☐ Measure iterations and robustness for different starting guesses.

Deliverables:

- `nonlin/root.h`, `nonlin/root.cpp`.
- Example programs illustrating method comparisons.

Tags: `Module:nonlin-root`, `Implementation`, `Experiment`

Phase 4 Card 3 – Implement Nonlinear System Solvers

Description: Solve small systems $F(\mathbf{x}) = 0$ using Newton-type methods.

Implementation Tasks:

- ☐ Implement Jacobian approximation via finite differences:
 - Wrap `diffint::deriv` for multivariate functions.
- ☐ Implement a Newton system solver:
 - At each iteration, solve $J(\mathbf{x}_k)\Delta\mathbf{x} = -F(\mathbf{x}_k)$ using `linalg::`.
- ☐ Implement simple globalisation strategies:
 - Damped steps or basic line search to improve robustness.

Experiment Tasks:

- ☐ Test on simple nonlinear systems (e.g., intersections of circles, small mechanical systems).
- ☐ Track convergence behavior for different initial guesses.

Deliverables:

- `nonlin/system.h`, `nonlin/system.cpp`.
- Example programs showing convergence and failure cases.

Tags: `Module:nonlin-root`, `Module:linalg`, `Implementation`, `Experiment`

Phase 5 – Linear Algebra & Optimization

Phase 5 Overview – Linear Algebra & Optimization

Goal: Build the linear algebra backbone and basic optimization algorithms used by many calculus applications (ODE, PDE, fitting).

Primary Sources:

- Numerical Recipes:
 - Chapter 2: solution of linear algebraic equations.
 - Chapter 10: minimization or maximization of functions.

Module Tie-ins:

- `linalg::` (linear algebra).
- `optim::` (optimization).

Exit Criteria:

- You can solve small dense systems and simple least-squares problems.
- You can perform basic 1D and multidimensional optimization.

Phase 5 Card 1 – Read Linear System Solvers

Description: Understand practical algorithms for solving $A\mathbf{x} = \mathbf{b}$.

Reading Tasks:

- Numerical Recipes, sections 2.0–2.4:
 - LU decomposition and Gaussian elimination.
 - Banded systems and conditioning notes.

Notes Deliverable:

- Short summary of:
 - When LU is appropriate vs. Cholesky.
 - The role of pivoting and conditioning.

Tags: Reading, Book:NR, Module:linalg

Phase 5 Card 2 – Implement Linear Algebra Core

Description: Implement key linear algebra routines.

Implementation Tasks:

- ☐ Implement a small dense matrix and vector type, or wrap an existing library with a thin façade.
- ☐ Implement LU decomposition with partial pivoting.
- ☐ Implement a solver using LU factors for multiple right-hand sides.
- ☐ Implement Cholesky decomposition for symmetric positive-definite matrices.

Experiment Tasks:

- ☐ Test on small random systems and known test matrices.
- ☐ Compare residuals for different methods and confirm numerical stability.

Deliverables:

- `linalg/linalg.h`, `linalg/linalg.cpp`.
- Unit tests for LU and Cholesky solvers.

Tags: `Module:linalg`, `Implementation`, `Experiment`

Phase 5 Card 3 – Read Scalar & Multidimensional Optimization

Description: Review core ideas in 1D and multidimensional optimization.

Reading Tasks:

- Numerical Recipes, sections 10.0–10.4:
 - 1D line searches.
 - Simple multidimensional methods.

Notes Deliverable:

- Summary of:
 - Golden-section search and Brent-like methods.
 - Basic gradient-based methods and convergence criteria.

Tags: Reading, Book:NR, Module:optim

Phase 5 Card 4 – Implement Optimization Routines

Description: Implement basic 1D and multidimensional optimization algorithms.

Implementation Tasks:

- ☐ 1D minimization:
 - Golden-section search.
 - Brent-type method for robustness.
- ☐ Multidimensional:
 - Gradient descent with line search.
 - Optionally conjugate gradient or quasi-Newton variant.

Experiment Tasks:

- ☐ Run on benchmark functions:
 - Quadratic bowls.
 - Rosenbrock function.
- ☐ Track iteration counts, convergence behavior, and sensitivity to starting guess.

Deliverables:

- `optim/optim.h`, `optim/optim.cpp`.
- Example programs visualizing convergence trajectories (e.g., contour plots with paths).

Tags: `Module:optim`, `Implementation`, `Experiment`

Phase 6 – ODEs & PDEs (Dynamics & Fields)

Phase 6 Overview – ODEs & PDEs

Goal: Use everything above to solve dynamical systems (ODEs) and simple PDEs.

Primary Sources:

- Numerical Recipes:
 - Chapter 17: integration of ODEs.
 - Chapters 18 and 20: boundary value problems and PDEs (for stretch goals).

Module Tie-ins:

- `ode::ivp`, `ode::bvp`.
- `pde::` (for simple finite-difference PDE solvers).

Exit Criteria:

- You can integrate basic ODEs with fixed and adaptive step sizes.
- You have at least one simple PDE (e.g., 1D heat equation) implemented and visualized.

Phase 6 Card 1 – Read ODE IVP Basics

Description: Understand explicit methods and adaptive step-size control.

Reading Tasks:

- Numerical Recipes, sections 17.0–17.2:
 - Runge–Kutta methods.
 - Step-size control strategies.

Notes Deliverable:

- Short summary of:
 - Local vs. global truncation error.
 - Stability considerations for explicit methods.

Tags: Reading, Book:NR, Module:ode

Phase 6 Card 2 – Implement ODE IVP Solvers

Description: Implement core IVP solvers and test them on classic examples.

Implementation Tasks:

☐ Implement:

- Explicit Euler step.
- RK4 step.
- Simple adaptive RK method (e.g., embedded RK pair).

☐ Design an API:

- `ode::solve_ivp(f, t0, y0, t_end, h_initial, options)` returning sampled trajectory.

Experiment Tasks:

☐ Test on:

- Exponential decay.
- Harmonic oscillator.
- Simple nonlinear systems.

☐ Plot solution trajectories and compare against analytic solutions where available.

Deliverables:

- `ode/ivp.h`, `ode/ivp.cpp`.
- Example plots of ODE solutions.

Tags: Module:ode, Implementation, Experiment

Phase 6 Card 3 – Read Stiff ODEs & Multistep Methods

Description: Understand the issues around stiffness and multistep approaches.

Reading Tasks:

- Numerical Recipes, sections 17.5–17.6:
 - Stiff ODEs.
 - Multistep methods.

Notes Deliverable:

- Short summary of:
 - What stiffness is and why explicit methods fail.
 - Basic idea of implicit methods and stability regions.

Tags: Reading, Book:NR, Module:ode

Phase 6 Card 4 – Implement Simple Stiff ODE Solver

Description: Implement a basic implicit scheme using your linear algebra module.

Implementation Tasks:

- ☐ Implement implicit Euler step:
 - Use Newton iteration to solve the implicit equation at each step.
- ☐ Reuse `linalg::` and `nonlin::` modules.

Experiment Tasks:

- ☐ Test on stiff problems (e.g., simple reaction equations).
- ☐ Compare explicit vs. implicit schemes and illustrate instability vs. stability.

Deliverables:

- Extension of `ode/ivp.*` or a separate `ode/stiff.*`.
- Plots showing behavior on stiff vs. non-stiff examples.

Tags: `Module:ode`, `Module:linalg`, `Module:nonlin-root`, `Implementation`, `Experiment`

Phase 6 Card 5 – Read PDE Overview & Implement 1D Heat Equation

Description: Take a first step into PDEs with a finite-difference 1D heat equation.

Reading Tasks:

- ☐ Numerical Recipes, sections 20.0–20.2:
 - Flux-conservative and diffusive PDEs.

Implementation Tasks:

- ☐ Discretize the 1D heat equation with:
 - Explicit scheme (forward Euler in time, central differences in space).
 - Implicit scheme if time allows.
- ☐ Use your linear algebra module for the implicit solves.

Experiment Tasks:

- ☐ Visualize temperature distribution over time.
- ☐ Compare stability and accuracy of explicit vs. implicit schemes.

Deliverables:

- `pde/heat1d.h`, `pde/heat1d.cpp`.
- Plots or animations of heat diffusion.

Tags: `Module:pde`, `Module:linalg`, `Implementation`, `Experiment`

Phase 7 – Random Numbers & Monte Carlo

Phase 7 Overview – Random Numbers & Monte Carlo

Goal: Use random numbers to drive Monte Carlo integration and stochastic simulations.

Primary Sources:

- TAOCP Vol. 2, Chapter 3: random numbers.
- Numerical Recipes, Chapter 7: random numbers and Monte Carlo.

Module Tie-ins:

- `rand::core`.
- `diffint::quad` (Monte Carlo as another integration approach).

Exit Criteria:

- You have a solid uniform RNG and basic distribution helpers.
- You can implement and compare Monte Carlo integration with deterministic quadrature.

Phase 7 Card 1 – Read PRNG Theory & Quality

Description: Understand the theoretical background for random number generation.

Reading Tasks:

- TAOCP Vol. 2, sections 3.1–3.3:
 - Linear congruential generators and other PRNGs.
 - Statistical tests and randomness criteria.
- Numerical Recipes, sections 7.0–7.4:
 - Practical PRNGs and basic tests.

Notes Deliverable:

- Brief notes on:
 - Why naive generators fail.
 - Key properties of good RNGs (period, equidistribution).

Tags: Reading, Book:TAOCP2, Book:NR, Module:rand

Phase 7 Card 2 – Implement Core RNG Module

Description: Implement uniform PRNGs and common distributions.

Implementation Tasks:

- ☐ Implement a high-quality uniform RNG (or wrap the C++ standard library in a controlled way).
- ☐ Provide:
 - `rand::uniform()`, `rand::normal()`, `rand::exponential()`, etc.
- ☐ Support seeding and independent streams.

Experiment Tasks:

- ☐ Perform basic statistical checks:
 - Histograms for various distributions.
 - Simple correlation and autocorrelation checks.

Deliverables:

- `rand/rand.h`, `rand/rand.cpp`.
- Small test programs visualizing distribution histograms.

Tags: `Module:rand`, `Implementation`, `Experiment`

Phase 7 Card 3 – Implement Monte Carlo Integrators

Description: Use your RNG to implement Monte Carlo integration.

Implementation Tasks:

- ☐ Implement simple Monte Carlo integrators:
 - `mc_integrate(f, domain, n_samples)`.
- ☐ Optionally add quasi-random sequences (e.g., Sobol or Halton).

Experiment Tasks:

- ☐ Compare Monte Carlo vs. deterministic quadrature from Phase 3:
 - Error vs. number of samples.
 - When Monte Carlo is preferable (e.g., higher-dimensional integrals).

Deliverables:

- `diffint/mc_quad.h`, `diffint/mc_quad.cpp` or integrated into `diffint::quad`.
- Plots comparing convergence rates.

Tags: `Module:rand`, `Module:diffint-quad`, `Implementation`, `Experiment`

Phase 8 – Capstone Projects

Phase 8 Overview – Capstone Pipelines

Goal: Execute small end-to-end projects that exercise multiple modules at once.

Capstone Themes:

- Nonlinear boundary-value ODE problems.
- PDE-based models coupled with optimization.

Exit Criteria:

- At least one nontrivial project is fully implemented, tested, and documented.
- You can explain how each module participates in the pipeline.

Phase 8 Card 1 – Capstone: Nonlinear Boundary-Value ODE

Description: Couple root finding, quadrature, and ODE solvers to handle a nonlinear BVP.

Pipeline Sketch:

- Model a simple physical or mathematical system (e.g., nonlinear beam, shooting method BVP).
- Use:
 - `ode::ivp` for shooting.
 - `nonlin::root` for matching boundary conditions.
 - `diffint::quad` if necessary for quantities defined by integrals.

Tasks:

- ☐ Define the differential equation and boundary conditions.
- ☐ Implement a shooting method:
 - Convert BVP to IVP.
 - Use root finding to adjust initial conditions.
- ☐ Validate against known or reference solutions if available.

Deliverables:

- An `examples/bvp_capstone.cpp` (or similar) program.
- A short write-up (1–2 pages) explaining model, methods, and results.

Tags: `Module:ode`, `Module:nonlin-root`, `Module:diffint-quad`, `Capstone`

Phase 8 Card 2 – Capstone: PDE + Optimization

Description: Combine PDE solving with parameter optimization.

Pipeline Sketch:

- Choose a simple steady-state PDE model (e.g., Laplace or Poisson).
- Introduce a parameter to be fitted (e.g., diffusion coefficient, source term amplitude).
- Use:
 - `pde::` for discretization and solution.
 - `optim::` to fit the parameter to synthetic or real data.
 - `stats::` (if implemented) to evaluate goodness of fit.

Tasks:

- ☐ Implement the PDE solver for the chosen model.
- ☐ Define an objective function measuring mismatch between solution and data.
- ☐ Optimize the parameter using methods from `optim::`.
- ☐ Analyze sensitivity to noise and initial guesses.

Deliverables:

- An `examples/pde_optim_capstone.cpp` (or similar) program.
- A brief report summarizing model, numerical methods, and optimization results.

Tags: `Module:pde`, `Module:optim`, `Module:stats`, `Capstone`

Module Reference (Quick Mapping)

Module `core::fp` – Floating-Point & Basic Arithmetic

Responsibilities:

- Provide floating-point utilities: `ulp`, `nearly_equal`.
- Robust summation and dot-product routines.
- Error metrics: absolute, relative, norms.

Book Mapping:

- TAOCP Vol. 2, Chapter 4 (arithmetic, floating-point).
- Numerical Recipes, Chapter 1 (error, accuracy, stability).

Module core::poly – Polynomial & Power-Series Arithmetic

Responsibilities:

- Represent polynomials and power series.
- Implement Horner evaluation, addition, multiplication, composition.
- Support Chebyshev and other polynomial-based approximations.

Book Mapping:

- TAOCP Vol. 2, sections 4.6–4.7 (polynomials, power series).
- Numerical Recipes, section 5.1 and 5.8–5.12 (polynomials, Chebyshev methods).

Module `rand::core` – Random Numbers & Distributions

Responsibilities:

- High-quality uniform PRNGs.
- Transformations to normal, exponential, and other distributions.
- Quasi-random sequences for Monte Carlo.

Book Mapping:

- TAOCP Vol. 2, Chapter 3 (random numbers).
- Numerical Recipes, Chapter 7 (random numbers and Monte Carlo).

Module `interp::` – Interpolation & Approximation

Responsibilities:

- Table lookup and interpolation in 1D (and later multidim).
- Polynomial, rational, spline, and Chebyshev interpolation.

Book Mapping:

- TAOCP Vol. 2, sections 4.6–4.7 (as algebraic backbone).
- Numerical Recipes, Chapter 3 and sections 5.8–5.10 (interpolation, Chebyshev).

Module `diffint::deriv` – Numerical Differentiation

Responsibilities:

- Finite-difference derivatives (forward, backward, central, higher order).
- Step-size selection and error modeling.
- Optional Richardson extrapolation.

Book Mapping:

- Numerical Recipes, section 5.7 (numerical derivatives).

Module `diffint::quad` – Numerical Integration & Monte Carlo

Responsibilities:

- 1D quadrature: trapezoid, Simpson, Romberg.
- Gaussian and adaptive quadrature.
- Multidimensional and Monte Carlo integration (ties to `rand::core`).

Book Mapping:

- Numerical Recipes, Chapter 4 (integration of functions).
- Numerical Recipes, sections 7.7–7.9 (Monte Carlo integration).

Module 1inalg:: – Linear Algebra Core

Responsibilities:

- Dense linear systems: LU, Cholesky, possibly QR/SVD.
- Banded and special matrices.
- Supporting routines for eigenproblems as needed.

Book Mapping:

- Numerical Recipes, Chapter 2 (linear equations).
- Numerical Recipes, Chapter 11 (eigensystems), if used.

Module `nonlin::root` – Root Finding & Nonlinear Systems

Responsibilities:

- 1D root solvers: bisection, secant, Brent, Newton.
- Nonlinear systems via Newton and globalized variants.

Book Mapping:

- Numerical Recipes, Chapter 9 (root finding and nonlinear systems).

Module `optim::` – Optimization & Minimization

Responsibilities:

- 1D minimization: golden-section, Brent.
- Multidimensional unconstrained optimization (gradient-based or simplex methods).

Book Mapping:

- Numerical Recipes, Chapter 10 (minimization or maximization of functions).

Module spectral:: – FFT & Spectral Tools

Responsibilities:

- FFT and inverse FFT.
- Spectral differentiation/integration.
- Convolution and filtering primitives.

Book Mapping:

- Numerical Recipes, Chapters 12–13 (FFT and spectral applications).

Module `ode::ivp`, `ode::bvp` – Ordinary Differential Equations

Responsibilities:

- IVP solvers: explicit/implicit, adaptive, stiff and non-stiff.
- BVP solvers: shooting methods, relaxation methods.

Book Mapping:

- Numerical Recipes, Chapters 17–18 (ODEs and BVPs).

Module `pde::` – Partial Differential Equations

Responsibilities:

- Finite-difference solvers for simple PDEs (1D/2D).
- Explicit/implicit schemes, stability helpers, and boundary conditions.

Book Mapping:

- Numerical Recipes, Chapter 20 (PDEs).

Module stats:: – Statistical Tools & Error Modeling

Responsibilities:

- Descriptive statistics and correlation.
- Least squares and error/convergence analysis for experiments.

Book Mapping:

- Numerical Recipes, Chapters 14–15 (statistics and data modeling).