Fundamentals of Simulation Methods – Exam Sheet

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1 Issues of floating point math

- common problems: **overflow** and **round-off errors**
- **two's complement**: *most significant bit* (MSB) (a.k.a. sign bit s) flags negative numbers
- floating point representations have a **base** β ($\beta = 2$ in IEEE standard), **precision** p (a.k.a *mantissa*), and **exponent** e
  - representation not unique, shifting exponent *and* mantissa can give same number multiple times; solution: *normalization*, i.e. leading digit before the point always 1
  - number in exponent E stored with *bias* b (hence E always positive as opposed to two's complement), e.g. $e = E - 127$ for floats
- in general, value f of IEEE float given by $f = (-1)^s\big(1 + \frac{M}{2^p}\big) \cdot 2^{E-b}$
- **machine precision**: smallest increment in mantissa, $\epsilon_m = \frac{1}{2^p}$
  - pitfall: $a + b = a$ even for $b \neq 0$ if $|b| < \epsilon_m \ |a|$

2 Integration of ordinary differential equations

- we seek solution $\boldsymbol{y}(t)$ to eq. of the form $\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}t} = \boldsymbol{f}(\boldsymbol{y}, t)$ subject to boundary condition, most commonly *initial value problem* (IVP)
- forward or **explicit Euler method**: $\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + \boldsymbol{f}(\boldsymbol{y}_n)\Delta t + \mathcal{O}_s(\Delta t^2)$
  - simplest approach, but only first-order accurate $\mathcal{O}_s(\Delta t^2)$ and unstable for large stepsize Δt
  - explicit because r.h.s. depends only on known quantities
- backward or **implicit Euler method**: $\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + \boldsymbol{f}(\boldsymbol{y}_{n+1})\Delta t$
  - excellent stability, hence useful for *stiff eqs.*, but still inaccurate for large Δt
  - often involves root-finding of nonlinear eq., numerically expensive
- **implicit midpoint rule**: $\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + \boldsymbol{f}\big(\frac{\boldsymbol{y}_n + \boldsymbol{y}_{n+1}}{2}\big)\Delta t + \mathcal{O}_s(\Delta t^3)$
  - second-order accurate but implicit so difficult in practice
- **Runge-Kutta methods**: derive from exact solution $\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + \int_{t_n}^{t_{n+1}} \boldsymbol{f}(\boldsymbol{y}(t))\,\mathrm{d}t$ by approximating integral with trapezoidal rule:

$$\begin{aligned} \boldsymbol{k}_1 = \boldsymbol{f}(\boldsymbol{y}_n, t_n), \quad \boldsymbol{k}_2 = \boldsymbol{f}(\boldsymbol{y}_n + \boldsymbol{k}_1\Delta t, t_{n+1}), \\ \boldsymbol{y}_{n+1} = \boldsymbol{y}_n + \frac{1}{2}(\boldsymbol{k}_1 + \boldsymbol{k}_2)\Delta t + \mathcal{O}_s(\Delta t^3) \end{aligned} \tag{1}$$

  - a.k.a. predictor-corrector scheme, $\boldsymbol{k}_1$ = predictor, $\boldsymbol{k}_2$ = corrector
  - 2nd-order accurate, higher-order schemes exist, e.g. RK-4:

$$\begin{aligned} \boldsymbol{k}_1 &= \boldsymbol{f}(\boldsymbol{y}_n, t_n), \quad \boldsymbol{k}_2 = \boldsymbol{f}\left(\boldsymbol{y}_n + \boldsymbol{k}_1\frac{\Delta t}{2}, t_n + \frac{\Delta t}{2}\right), \\ \boldsymbol{k}_3 &= \boldsymbol{f}\left(\boldsymbol{y}_n + \boldsymbol{k}_2\frac{\Delta t}{2}, t_n + \frac{\Delta t}{2}\right), \\ \boldsymbol{k}_4 &= \boldsymbol{f}(\boldsymbol{y}_n + \boldsymbol{k}_3\Delta t, t_n + \Delta t), \\ \boldsymbol{y}_{n+1} &= \boldsymbol{y}_n + \frac{1}{6}(\boldsymbol{k}_1 + 2\boldsymbol{k}_2 + 2\boldsymbol{k}_3 + \boldsymbol{k}_4)\Delta t + \mathcal{O}_s(\Delta t^5) \end{aligned} \tag{2}$$

- **adaptive step size**: achieve optimum compromise between accuracy, efficiency and stability by e.g. estimating error based on difference between one full step and two half-steps, define local error bounds, increase stepsize if below, decrease if above
- **reduction to 1st order**: bring higher-order diff. eqs. into standard form, e.g. cast $\ddot{\boldsymbol{x}} = \boldsymbol{f}(x)$ into $\dot{\boldsymbol{y}} = \tilde{\boldsymbol{f}}(\boldsymbol{y})$ by defining $\boldsymbol{y} = (\boldsymbol{x}, \dot{\boldsymbol{x}})$ and $\tilde{\boldsymbol{f}} = (\dot{\boldsymbol{x}}, \boldsymbol{f}(\boldsymbol{x}))$, then apply e.g. Runge-Kutta
- **leapfrog**: very simple alternative in above case; define $\boldsymbol{v} \equiv \dot{\boldsymbol{x}}$, then

$$\begin{aligned} \boldsymbol{x}_{n+1} &= \boldsymbol{x}_n + \boldsymbol{v}_{n+\frac{1}{2}}\Delta t, \\ \boldsymbol{v}_{n+\frac{3}{2}} &= \boldsymbol{v}_{n+\frac{1}{2}} + \boldsymbol{f}(\boldsymbol{x}_{n+1})\Delta t \end{aligned} \tag{3}$$

  - 2nd-order accurate and requires only one evaluation per step
  - name leapfrog due to interleaved advances of position and velocity
  - better than higher-order schemes on some systems due to being symplectic and time-reversible
- **symplectic integrator**: structure-preserving method that observes special properties of Hamiltonian systems, e.g. energy and phase-space volume conservation (*Liouville theorem*)
  - let $\omega : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, $\omega(\xi, \eta) = A_{P(\xi \times \eta)}$ give area of parallelogram $P(\xi \times \eta)$ spanned by $\xi, \eta \in \mathbb{R}^d$; then linear map $F : \mathbb{R}^d \to \mathbb{R}^d$ is symplectic if $\omega(F\xi, F\eta) = \omega(\xi, \eta)$
  - a differentiable map $g : U \to \mathbb{R}^d$ is symplectic if its Jacobian is symplectic everywhere
  - **Poincaré's theorem**: time evolution generated by a Hamiltonian in phase-space is a symplectic transformation

3 Collisionless particle systems

- central idea: describe large-N-body system as small-N system by grouping real particles into fiducial macro particles
  - for gravity, the e.o.m.s with (numerical) *softening length* ϵ are $\ddot{\boldsymbol{x}}_i = -\boldsymbol{\nabla}\Phi(\boldsymbol{x}_i)$, $\Phi(\boldsymbol{x}) = -G\sum_{j=1}^{N} \frac{m_j}{\sqrt{(\boldsymbol{x} - \boldsymbol{x}_j)^2 + \epsilon^2}}$
  - purpose of ϵ: prevent (highly correlated) bound states (requires $\langle v^2 \rangle \gg \frac{Gm}{\epsilon}$), avoid numerical expense of large angle scattering in singular potential; ϵ introduces smallest resolved length scale
- examples: electrons in plasma, globular star clusters, stars in a galaxy, dark matter (all are also *uncorrelated* to good approx.)

4 Tree algorithms

- more spec. **hierarchical multipole algorithms** enable fast, approximate force calculations for N-body systems (see Section 3)
  - group hierarchy organized in *tree-like* data structure
  - scale with $\mathcal{O}(N \ln N)$, whereas *direct summation* is $\mathcal{O}(N^2)$
- central idea: use multipole expansion for (grav.) potential created by group of distant particles rather than sum up forces individually
  - *monopole*: $M = \sum_{i=1}^{N} m_i$, *quadrupole*: $Q_{ij} = \sum_{k=1}^{N} m_k \Big[3(\boldsymbol{s} - \boldsymbol{x}_k)_i (\boldsymbol{s} - \boldsymbol{x}_k)_j - \delta_{ij}(\boldsymbol{s} - \boldsymbol{x}_k)^2\Big]$, where $\boldsymbol{s}$ points to c.o.m.
  - dipole vanishes when expansion is done relative to c.o.m.
  - expansion accurate if $\frac{r}{d} \leq \theta$ for chosen **opening angle** θ; r, d radius and distance of particle group

5 The particle-mesh technique

- alternative to tree algorithms, used in MD and astrophysics
- 1. construct density field ρ on suitable auxiliary mesh 2. compute potential Φ on mesh by solving Poisson's eq. 3.

calculate force field $\boldsymbol{F}$ from potential 4. calculate forces $\boldsymbol{F}_i$ at original particle positions

2. mass assignment onto auxiliary mesh via *nearest grid point* (NGP), *clouds in cell* (CIC), or *triangular shaped clouds* (TSC)
   - NGP: density jumps discont. when particle crosses cell boundary, resulting force piece-wise constant; CIC: force piece-wise linear and continuous, but derivative jumps; TSC: both force and its derivative smooth
3. solve Poisson's eq. $\Delta\Phi = 4\pi G\rho$ either with Fourier transform (Section 6) or iteratively (Section 7)
4. calculate acceleration $\boldsymbol{a} = -\boldsymbol{\nabla}\Phi$ with **finite differencing**, e.g. $a_x(i,j,k) = -\frac{1}{2h}\left[\Phi(i+1,j,k) - \Phi(i-1,j,k)\right] + \mathcal{O}(h^2)$ or with *larger stencil* to reduce truncation error below $\mathcal{O}(h^2)$
5. interpolate from mesh to particles: $\boldsymbol{F}_i(\boldsymbol{x}_i) = m\sum_{\boldsymbol{p}} \boldsymbol{a}_{\boldsymbol{p}} W(\boldsymbol{x}_i - \boldsymbol{x}_{\boldsymbol{p}})$, where sum runs over auxiliary mesh cells $\boldsymbol{p} = (i,j,k)$
   - W *same* assignment kernel as used in density construction, ensures vanishing *self-force* and pairwise antisymmetric forces

6 Force calculation with Fourier transform techniques

- tool for solving certain PDEs, e.g. Poisson's eq. $\Delta\Phi = 4\pi G\rho$; sol. $\Phi(\boldsymbol{x}) = -G\int \frac{\rho(\boldsymbol{x}')\,\mathrm{d}\boldsymbol{x}'}{|\boldsymbol{x}-\boldsymbol{x}'|} = \rho \star g$ is convolution of ρ with $g(\boldsymbol{x}) = -\frac{G}{|\boldsymbol{x}|}$
- **convolution thm.**: $\mathcal{F}(f\star g) = \mathcal{F}(f)\cdot\mathcal{F}(g) \Rightarrow \Phi = \mathcal{F}^{-1}[\mathcal{F}(\rho)\cdot\mathcal{F}(g)]$
- in practice, to solve this requires assuming *periodic* b.c. in box of size L, gives finite discrete $\boldsymbol{k}$-space so we can apply (*discrete*) *fast Fourier transform* (FFT), scales with $\mathcal{O}(N\ln N)$
- for nonperiodic problems: **zero-padding** constructs mesh s.t. sources lives only in one quarter (in 2D), rest of mesh is zeroed-out

7 Iterative solvers and the multigrid technique

- ansatz: discretize Φ on regular N-point mesh with spacing h so Poisson's eq. at cell $i \in \{0,...,N-1\}$ is $\frac{\Phi_{i+1}-2\Phi_i+\Phi_{i-1}}{h^2} = 4\pi G\rho_i$
- above can be cast into set of N linear eqs. $\mathbf{A}\boldsymbol{\Phi} = \boldsymbol{b}$ with $\mathbf{A}$ stencil matrix, $\boldsymbol{b} = 4\pi G(\rho_0,...,\rho_{N-1})$; analytic. solvable with Gauss elimination, but not feasible for large N (scales $\mathcal{O}(N^3)$)
- use **Jacobi** or **Gauss-Seidel iteration** instead by decomposing $\mathbf{A} = \mathbf{D} - \mathbf{U} - \mathbf{L}$, yields Jac. update formula $\Phi_i^{(n+1)} = \frac{1}{2}\left(\Phi_{i+1}^{(n)} + \Phi_{i-1}^{(n)} - 4\pi G h^2\rho_i\right)$ or GS $\boldsymbol{\Phi}^{(n+1)} = \mathbf{D}^{-1}\left[\mathbf{U}\boldsymbol{\Phi}^{(n)} + \mathbf{L}\boldsymbol{\Phi}^{(n+1)} + \boldsymbol{b}\right]$
  - GS looks like, but is not implicit formula; no values of $\boldsymbol{\Phi}^{(n+1)}$ are needed, because $\mathbf{L}$ has only elements below diagonal
  - GS makes use of updated values immediately, $\approx$ twice as fast as Jacobi, but has to be solved sequentially $\Rightarrow$ not parallelizable
- **red-black ordering**: some update rules allow decomposition of cells into disjoint sets whose update depends only on cells from other set(s), e.g. for Poisson's eq.: chessboard pattern
- convergence of Jac. and GS often '*stalls*'; high-ν errors die quickly, but low-ν, high-λ errors slowly; reason: per step, information travels only one stencil length, convergence needs several sweeps
- solution: **multigrid**; central idea: go to coarser mesh, compute improved initial guess, helps speed up convergence on fine grid
  - because multigrid operates on coarser grid for most of time, it is *much* faster, cheaper than Jac. and GS
  - fine $\rightarrow$ coarse and back requires restriction and prolongation operators; in 1D: restr. with $\mathbf{I}_h^{2h} = \left[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right]$, prol. with $\mathbf{I}_{2h}^{h} =]\frac{1}{2}, 1, \frac{1}{2}[$

8 Molecular dynamics simulations

- aim: simulate atoms, molecules, proteins, etc. in *microscopic* detail over relevant timespan to determine mech., electr., etc. properties
- important point: uses Newton's *classical* e.o.m.s, based on approximation of inter- and/or intra-molecular forces, force laws may be empirical or quantum mechanically derived
- intimately connected to stat. mech.: precise microstate unimportant, interested in *ensemble averages* of macro. var. T, P, ρ, etc.
- **ergodic hypothesis**: postulates ensemble avr. = time avr., thus evolve MD sim. to reach equilibrium, then measure time avr. $\overline{A} = \lim_{\tau\to\infty}\frac{1}{\tau}\int_{t_0}^{t_0+\tau} A(\Gamma(t))\,\mathrm{d}t$ of macros. quantity $A(\Gamma)$, fct. of microstate Γ
- **finite range interactions**: molecules interact only over short range, e.g. *Lennard-Jones potential* $V(r) = 4\epsilon\left[\frac{\sigma^{12}}{r^{12}} - \frac{\sigma^6}{r^6}\right] \Rightarrow$ introduce cutoff $V_c(r) = 0$ for $r > r_c$ and search grid, ignore particles in cells farther than r_c; reduces scaling from $\mathcal{O}(N^2)$ to $\mathcal{O}(N)$

9 Basic gas dynamics

- **Euler eqs.**: describe continuity of mass, momentum, energy during dynamics of ideal, i.e. frictionless, gas

$$\begin{aligned}\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\boldsymbol{v}) &= 0,\\ \frac{\partial\rho\boldsymbol{v}}{\partial t} + \boldsymbol{\nabla}(\rho\boldsymbol{v}^2 + P) &= 0,\\ \frac{\partial\rho e}{\partial t} + \boldsymbol{\nabla}\cdot[(\rho e + P)\boldsymbol{v}] &= 0\end{aligned} \tag{4}$$

  with total energy (per unit mass) $e = u + \frac{\boldsymbol{v}^2}{2}$, u thermal energy; closed by eq. of state $P = (\gamma-1)\rho u$ with adiabatic index $\gamma = C_P/C_V$
- **Navier-Stokes eqs.**: describe dynamics of real fluids with internal stress due to *viscosity* (dissipates relative motion into heat)

$$\begin{aligned}\frac{\partial\rho\boldsymbol{v}}{\partial t} + \boldsymbol{\nabla}(\rho\boldsymbol{v}^2 + P) &= \boldsymbol{\nabla}\boldsymbol{\Pi},\\ \frac{\partial\rho e}{\partial t} + \boldsymbol{\nabla}\cdot[(\rho e + P)\boldsymbol{v}] &= \boldsymbol{\nabla}(\boldsymbol{\Pi}\boldsymbol{v})\end{aligned} \tag{5}$$

  (continuity eq. identical to Euler) with viscous stress tensor (material property) $\boldsymbol{\Pi} = \eta\left[\boldsymbol{\nabla}\boldsymbol{v} + (\boldsymbol{\nabla}\boldsymbol{v})^{\mathrm{T}} - \frac{2}{3}(\boldsymbol{\nabla}\cdot\boldsymbol{v})\mathbb{1}\right] + \xi(\boldsymbol{\nabla}\cdot\boldsymbol{v})\mathbb{1}$, where η (ξ) scales traceless (diagonal) part, i.e. shear (bulk) viscosity
- **shocks**: hydro-flows can develop shock waves where density, velocity, temperature, specific entropy jump; typical for hyperbolic PDEs; shocks decelerate, compress and heat up fluid
  - differential form of Euler eqs. breaks down at discontinuity, (weak) integral formulation remains valid; assuming rest frame of shock ($v_s = 0$) and piece-wise constant states left/right leads to Rankine-Hugoniot jump cdts.

$$\begin{aligned}\rho v = \rho' v', \quad \rho v^2 + P = \rho' v'^2 + P',\\ (\rho e + P)v = (\rho' e' + P')v'\end{aligned} \tag{6}$$

  - presence of shock requires Mach number $\mathcal{M} = \frac{v}{c_s} > 1$, i.e. pre-shock gas streams supersonically into discontinuity, $c_s^2 = \frac{\gamma P}{\rho}$
- **fluid instabilities**: start with two phases (ρ_1, v_1), (ρ_2, v_2), gravity $\boldsymbol{g}$ in $-z$-direction, consider single pert. Fourier mode $\xi = \tilde{\xi}e^{i(kx-\omega t)}$

- **Rayleigh-Taylor**: $v_1 = v_2 = 0 \Rightarrow$ disp. rel. $\omega^2 = \frac{(\rho_2 - \rho_1)kg}{\rho_1 + \rho_2}$ (phase 1 on top); unstable solutions with $\mathrm{Im}(\omega) > 0$ exist for $\rho_1 > \rho_2$, i.e. heavy fluid on top of light one
- **Kelvin-Helmholtz**: $\boldsymbol{g = 0}$, i.e. pure shear flow $\Rightarrow \omega_{1,2} = k\frac{(\rho_1 v_1 + \rho_2 v_2)}{\rho_1 + \rho_2} \pm ik\frac{\sqrt{\rho_1 \rho_2}}{\rho_1 + \rho_2}\,|v_1 - v_2|$; $\mathrm{Im}(\omega) > 0$ always if $v_1 \neq v_2$, i.e. small perturbation at phase interface will grow rapidly into characteristic KH vortices (fluid turbulences)

10 Eulerian hydrodynamics

- important linear and homogeneous PDEs: *Laplace* $\Delta u = 0$, *heat conduction* $\partial_t u = \lambda^2 \Delta u$, *wave propagation* $\partial_t^2 u = c^2 \Delta u$
- classify 2nd-order linear PDEs $a\partial_x^2 u + b\partial_x \partial_y u + c\partial_y^2 u + d\partial_x u + e\partial_y u + fu = g$ according to $D = b^2 - 4ac$: $D < 0$ elliptic (static problems without time dependence), $D = 0$ parabolic (slowly changing processes, e.g. diffusion), $D > 0$ hyperbolic (dynamical processes that can develop discontinuities)
- **Riemann problem**: IVP for hyperbolic system of two (piece-wise constant) phases characterized at $t = 0$ by state vectors $\boldsymbol{U}_i = (\rho_i, P_i, \boldsymbol{v}_i)$, $i \in \{R, L\}$, task: evolve system for $t > 0$
  - (always present) *contact wave*: boundary between phases
  - may be sandwiched between *shock* and/or *rarefaction waves*
  - waves propagate with constant speed, fluid properties $(\rho^\star, P^\star, \boldsymbol{v}^\star)$ at $x = 0$ *constant in time* for $t > 0$
  - for $\boldsymbol{v}_L = \boldsymbol{v}_R = 0$, Riemann problem simplifies to *Sod shock tube*

11 Smoothed particle hydrodynamics

- (versatile mesh-free) technique to approximate fluid continuum dynamics through particles (interpolation points)
- advantages: 1. provides automatically adaptive spatial resolution and density 2. ensures conservation of energy, (angular) momentum, mass, entropy 3. Galilean invariant and advection-error-free 4. can deal with complicated geometries and large empty regions due to mesh-free nature 5. robust: does not produce negative ρ's and T's
- disadvantage: limited accuracy in multi-dim. flows, gives rise to velocity noise, degrades accuracy and leads to slow convergence

12 Finite element methods

- for solving PDEs, good at flexible geometries, odd b.c., allows spatially variable resolution
- central idea: 1. divide domain into smaller regions (*elements*) containing points (*nodes*), possible boundaries: segments (1D), triangles (2D), tetrahedra (3D) 2. choose (linearly indep.) basis fcts. (called *shape fcts.*) to describe solution on each element, e.g. polynomial basis 3. n coefficients in element expansion require n nodes to uniquely specify *reconstruction* inside element

13 Monte Carlo Techniques

- lie at the heart of *stochastic simulations*
- **error** of Monte Carlo integration I_N given by width σ_N of its probability distribution $P_N(I_N)$; always a Gaussian according to **central limit theorem** so $\sigma_N = V\sqrt{\frac{\langle f^2\rangle - \langle f\rangle^2}{N}}$
  - $\propto 1/\sqrt{N}$, irrespective of dimensionality d of integration domain
- **importance sampling**: choose random points preferentially around peaks of function to be integrated
- virtues of **pseudo-random number generators**: repeatability, randomness, speed, portability, long period, insensitivity to seed
- **exact inversion**: method for creating nonuniform PDF $p(y)$ from uniform distr. $q(x) = \frac{1}{b-a}$ over the interval $[a, b]$; uses conservation of probability to equate respective CDFs

$$Q(x) = \int_{-\infty}^{x} q(x')\,\mathrm{d}x' \stackrel{!}{=} \int_{-\infty}^{y} p(y')\,\mathrm{d}y' = P(y) \qquad (7)$$

- **rejection method**: used to create uninvertible random number distr. $p(y)$ from distr. $f(y) \geq p(y)$ we *can* produce
  - 1. generate y from $f(y)$ 2. generate z from uniform distr. with bounds $0 \leq z < f(y)$ 3. if $z \leq p(y)$, return y as sample value 4. else reject trial value for y and start again
- **Markov chain**: discrete sequence of states x_i generated by *Markov process* f which must 1. preserve eq. distr. $p_{\mathrm{eq}}(x)$ of stochastic process 2. starting from x, be able to reach any other state x' (*ergodicity*)
- **Metropolis-Hastings algorithm**: 1. from current state x, propose new state x' with proposal probability $q(x \to x')$ 2. accept proposed move with probability given by *Hastings ratio* $r = \min\left(1, \frac{p(x')q(x' \to x)}{p(x)q(x \to x')}\right)$ 3. otherwise reject x' and add x to Markov chain (again)
  - fulfills *detailed balance*: $p_{\mathrm{eq}}(x)W_f(x \to x') \stackrel{\checkmark}{=} p_{\mathrm{eq}}(x')W_f(x' \to x)$