Simulation and High-Performance Computing Part 2: Time-Stepping Methods for Special Applications

Steffen Börm

Christian-Albrechts-Universität zu Kiel

September 28th, 2020

Leapfrog method

Goal: Accuracy of Runge's method with the computational work of Euler's.

Idea: As in Runge's method, use the central difference quotient

$$\frac{y(t+\delta)-y(t)}{\delta}\approx y'(t+\frac{\delta}{2})=f(t+\frac{\delta}{2},y(t+\frac{\delta}{2})),$$
$$y(t+\delta)\approx y(t)+\delta f(t+\frac{\delta}{2},y(t+\frac{\delta}{2})).$$

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Two-step method: Compute midpoint states also with the central difference quotient.

$$y(t + \frac{3}{2}\delta) \approx y(t + \frac{\delta}{2}) + \delta f(t + \delta, y(t + \delta)).$$

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Algorithm: Alternate between states at $t, t+\delta, t+2\delta, \ldots$ and midpoint states $t+\frac{\delta}{2}, t+\frac{3}{2}\delta, t+\frac{5}{2}\delta, \ldots$

Leapfrog algorithm

Time grid: Starting at time t_0 , let

$$t_k := t_0 + \delta k,$$
 $t_{k+1/2} := t_0 + \delta (k + \frac{1}{2}).$

Alternating computation of approximated states

$$\tilde{y}(t_0) := y(t_0),$$

$$\tilde{y}(t_{k+1}) := \tilde{y}(t_k) + \delta f(t_{k+1/2}, \tilde{y}(t_{k+1/2})),
\tilde{y}(t_{k+3/2}) := \tilde{y}(t_{k+1/2}) + \delta f(t_{k+1}, \tilde{y}(t_{k+1})).$$

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$$\begin{split} \widetilde{y}(t_0) &:= y(t_0), \\ \widetilde{y}(t_{1/2}) &:= y(t_0) + \frac{\delta}{2} f(t_0, y(t_0)), \\ \widetilde{y}(t_{k+1}) &:= \widetilde{y}(t_k) + \delta f(t_{k+1/2}, \widetilde{y}(t_{k+1/2})), \\ \widetilde{y}(t_{k+3/2}) &:= \widetilde{y}(t_{k+1/2}) + \delta f(t_{k+1}, \widetilde{y}(t_{k+1})). \end{split}$$

The first midpoint state is computed by Euler's method.

Leapfrog method: Implementation

Leapfrog method for the mass-spring system in C:

```
/* Use Euler's method for first midpoint state */
xm = x + 0.5 * delta * v;
vm = v - 0.5 * delta * c / m * x:
for(k=0; k< n; k++) {
 /* Update state */
 x += delta * vm:
 v = delta * c / m * xm:
  /* Update midpoint state */
 xm += delta * v;
 vm -= delta * c / m * x:
```

Leapfrog method: Improved implementation

Idea: For the mass-spring system, x'(t) depends only on v(t) and v'(t) depends only on x(t).

ightarrow Compute midpoint states only for the velocity.

```
/* Use Euler's method for first midpoint state */
vm = v - 0.5 * delta * c / m * x;

for(k=0; k<n; k++) {
    /* Update state */
    x += delta * vm;

    /* Update midpoint state */
    vm -= delta * c / m * x;
}</pre>
```

Result: Accuracy of Runge's method at the "price" of Euler's method.

Experiment: Leapfrog method for the mass-spring system

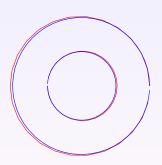
Approach: Start at t=0, perform successive timesteps to reach t=20.

	Euler		Runge		Leapfrog	
δ	error	ratio	error	ratio	error	ratio
1	1.0_{+3}		9.6+0		9.1_{-1}	
1/2	8.2 ₊₁	12.2	8.7_{-1}	11.0	2.0_{-1}	4.6
1/4	7.9_{+0}	10.4	1.9_{-1}	4.6	4.8_{-2}	4.2
1/8	1.3_{+0}	6.1	4.6_{-2}	4.1	1.2_{-2}	4.0
1/16	4.0_{-1}	3.3	1.2_{-2}	3.8	3.0_{-3}	4.0
1/32	1.6_{-1}	2.5	2.9_{-3}	4.1	7.4_{-4}	4.1
1/64	7.1_{-2}	2.3	7.4_{-4}	3.9	1.9_{-4}	3.9
1/128	3.4_2	2.1	1.9_{-4}	3.9	4.6_5	4.1
1/256	1.6_{-2}	2.1	4.6_{-5}	4.1	1.2_{-5}	3.8

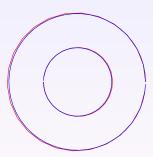
Observation: For this particular problem, the leapfrog method is more efficient and more accurate than Runge's method.

Experiment: Leapfrog for the gravity system

Runge's method with 25/50 timesteps.

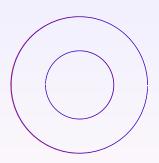


Leapfrog method with 25/50 timesteps.

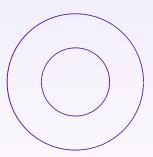


Experiment: Leapfrog for the gravity system

Runge's method with 50/100 timesteps.

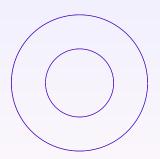


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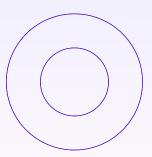


Experiment: Leapfrog for the gravity system

Runge's method with 100/200 timesteps.



Leapfrog method with 100/200 timesteps.



Example: $y'(t) = -\lambda y(t)$ with $\lambda > 0$, exact solution $y(t) = e^{-\lambda t}$.

Explicit Euler method takes the form

$$y(t + \delta) \approx y(t) - \delta \lambda y(t) = (1 - \delta \lambda)y(t).$$

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• Completely unrealistic oscillations if $2 < \delta \lambda$.

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- Oscillations with exponential decay if $1 < \delta \lambda < 2$.

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Observation:

- Completely unrealistic oscillations if $2 < \delta \lambda$.
- Oscillations with exponential decay if $1 < \delta \lambda < 2$.
- Proper behaviour only if $\delta \lambda < 1$.

Implicit Euler method

Backward difference quotient: Taylor expansion yields $\eta \in [t,t+\delta]$ with

$$y(t) = y(t+\delta) - \delta y'(t+\delta) + \frac{\delta^2}{2}y''(\eta),$$
$$\frac{y(t+\delta) - y(t)}{\delta} = y'(t+\delta) + \frac{\delta}{2}y''(\eta)$$

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Implicit Euler: Drop last term, use $y'(t + \delta) = f(t + \delta, y(t + \delta))$.

$$\tilde{y}(t+\delta) = y(t) + \delta f(t+\delta, \tilde{y}(t+\delta)).$$

Problem: Both sides depend on unknown future state $\tilde{y}(t+\delta)$.

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Model problem is linear, therefore easy to handle.

$$\tilde{y}(t+\delta) = y(t) - \delta\lambda\,\tilde{y}(t+\delta) \iff \tilde{y}(t+\delta) = \frac{1}{1+\delta\lambda}y(t)$$

Experiment: Explicit vs implicit Euler

Example:
$$y'(t) = -\lambda y(t)$$
, exact solution $y(t) = e^{-\lambda t}$.

Explicit Euler:

Implicit Euler:



Observation: At the same timestep size, the implicit method yields far more realistic results.

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Application: Parabolic and hyberbolic partial differential equations, e.g., heat or wave equations. \rightarrow Courant-Friedrichs-Levy condition.

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Example: Mass-spring system.

$$x'(t) = v(t), v'(t) = -\frac{c}{m}x(t).$$

Energy of the system consists of potential and kinetic energy.

$$E(t) := \frac{c}{2}x(t)^2 + \frac{m}{2}v(t)^2.$$

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= $c x(t)v(t) + m v(t) \left(-\frac{c}{m}\right)x(t) = 0.$

The total energy of the system is constant.

Explicit Euler method:

$$\tilde{E}(t+\delta) = \frac{c}{2}(x(t)+\delta v(t))^2 + \frac{m}{2}\left(v(t)-\delta \frac{c}{m}x(t)\right)^2$$

Explicit Euler method:

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Explicit Euler method: Total energy increased with each timestep.

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Implicit Euler method: Total energy decreased with each timestep.

$$\tilde{E}(t+\delta) = \frac{c}{2}(x(t)+\delta\,\tilde{v}(t+\delta))^2 + \frac{m}{2}\left(v(t)-\delta\,\frac{c}{m}\tilde{x}(t+\delta)\right)^2 \\
= E(t)-\delta^2\frac{c}{m}\tilde{E}(t+\delta) \le E(t).$$

Idea: Combine the explicit and the implicit Euler method.

$$\widetilde{y}_{ex}(t+\delta) := y(t) + \delta f(t, y(t)),$$

$$\widetilde{y}_{im}(t+\delta) := y(t) + \delta f(t+\delta, \widetilde{y}_{im}(t+\delta)),$$

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Mass-spring system: Solve linear equations

$$\tilde{x}(t+\delta) = x(t) + \frac{\delta}{2}(v(t) + \tilde{v}(t+\delta)),$$

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Mass-spring system: Solve linear equations to obtain explicit algorithm.

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Experiment: Euler vs Crank-Nicolson

Approach: Start at t = 0, perform successive timesteps to reach t = 10.

	Explicit		Implicit		Crank-Nic	
δ	error	ratio	error	ratio	error	ratio
1/2	8.4 ₊₀		7.3_{-1}		9.2_{-2}	
1/4	2.3_{+0}	3.7	5.6_{-1}	1.3	2.7_{-2}	3.4
1/8	7.7_{-1}	3.0	3.7_{-1}	1.5	7.0_{-3}	3.9
1/16	3.2_{-1}	2.4	2.2_{-1}	1.7	1.8_{-3}	4.0
1/32	1.4_{-1}	2.2	1.2_{-1}	1.8	4.4_{-4}	4.0
1/64	6.9_{-2}	2.1	6.3_{-2}	1.9	1.1_{-4}	4.0
1/128	3.4_2	2.0	3.2_{-2}	2.0	2.8_{-5}	4.0
1/256	1.7_{-2}	2.0	1.6_{-2}	2.0	6.9_{-6}	4.0
1/512	8.2_3	2.0	8.1_{-3}	2.0	$ 1.7_{-6} $	4.0

Observation: The Crank-Nicolson method is of second order.

Discrete conservation of energy

Crank-Nicolson for the mass-spring system:

$$\tilde{x}(t+\delta) = x(t) + \frac{\delta}{2}(v(t) + \tilde{v}(t+\delta)),$$

$$\tilde{v}(t+\delta) = v(t) - \frac{\delta}{2}\frac{c}{m}(x(t) + \tilde{x}(t+\delta))$$

Energy is preserved, since the third binomial equation yields

$$\tilde{E}(t+\delta)-E(t)=\frac{c}{2}(\tilde{x}(t+\delta)^2-x(t)^2)+\frac{m}{2}(\tilde{v}(t+\delta)^2-v(t)^2)=0.$$

Discrete conservation of energy

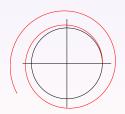
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Summary

Leapfrog method: Uses the central difference quotient, propagates midpoint states.

$$\begin{split} & ilde{y}(t+\delta) := ilde{y}(t) + \delta \, f(t+rac{\delta}{2}, ilde{y}(t+rac{\delta}{2})), \ & ilde{y}(t+rac{3}{2}\delta) pprox ilde{y}(t+rac{\delta}{2}) + \delta \, f(t+\delta, ilde{y}(t+\delta)). \end{split}$$

Implicit Euler method: Future state defined via fixed-point equation.

$$\tilde{y}(t+\delta) = y(t) + \delta f(t+\delta, \tilde{y}(t+\delta)).$$

Implicit methods are very useful for stiff equations.

Crank-Nicolson method: Provides conservation of energy, at least for the mass-spring system.

$$\tilde{y}(t+\delta) = y(t) + \frac{\delta}{2}(f(t,y(t)) + f(t+\delta,\tilde{y}(t+\delta)).$$