



High-Performance Numerical Integration in the Age of C++26

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High-Performance Numerical Integration in the Age of C++26

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Introduction

1 Introduction

2 Firs ts steps

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Starting with an example (in good old C++20)

What is this program doing?

```
1 // Preamble
2 #include <array>
3 #include <cmath>
4 #include <string>
5 #include <vector>
6 #include <iostream>
7 #include <limits>
8 // Main function
9 int main(int argc, char* argv[]) {
10     // Constants
11     using type = double;
12     constexpr type au = 149597870700.;
13     constexpr type year = 365.25 * 24 * 60 * 60;
14     constexpr type mpc = 1.E6 * (180 * 60 * 60 * au) / std::numbers::pi_v<type>;
15     // Parameters
16     const type h0 = (argc > 1) ? std::stod(argv[1]) : 0.677;
17     const type hubble_0 = h0 * 100 * 1000 / mpc;
18     const type omega_r0 = (argc > 2) ? std::stod(argv[2]) : (2.47E-5 * h0 * h0);
19     const type omega_m0 = (argc > 3) ? std::stod(argv[3]) : 0.311;
20     const type omega_l0 = (argc > 4) ? std::stod(argv[4]) : 0.689 - omega_r0;
21     const type omega_k0 = 1 - (omega_r0 + omega_m0 + omega_l0);
22     const type h = (argc > 5) ? std::stod(argv[5]) : (1.E3 * year);
23     const type a0 = (argc > 6) ? std::stod(argv[6]) : (1.);
24     // Computation
25     auto evolution = compute(hubble_0, omega_r0, omega_m0, omega_l0, omega_k0, h, a0);
26     // Output
27     std::cout << std::abs(evolution.back()[0] / (1.E9 * year)) << std::endl;
28     return 0;
29 }
```

Starting with an example (in good old C++20)

What is this program doing?

```
1 // Computation
2 template <class T>
3 constexpr auto compute(T hubble_0, T omega_r0, T omega_m0, T omega_l0, T omega_k0, T h, T a0) {
4     // Variables
5     T t = 0;
6     T a = a0;
7     // Output
8     std::vector<std::array<T, 2>> evolution;
9     evolution.reserve((static_cast<T>(1) / hubble_0) / h);
10    // Function to integrate
11    auto da_dt = [&](auto t, auto a) {
12        return a * hubble_0 * std::sqrt(
13            omega_r0 * std::pow(a, static_cast<T>(-4))
14            + omega_m0 * std::pow(a, static_cast<T>(-3))
15            + omega_k0 * std::pow(a, static_cast<T>(-2))
16            + omega_l0
17        );
18    };
19    // Computation
20    while (a > std::numeric_limits<T>::epsilon()) {
21        evolution.emplace_back(std::array<T, 2>{t, a});
22        a = a - h * da_dt(t, a);
23        t = t - h;
24    }
25    // Output
26    return evolution;
27 }
```

The output

13.7839

What's missing?

- A quantity and units library would be very (very) nice!

13.7839 billion years

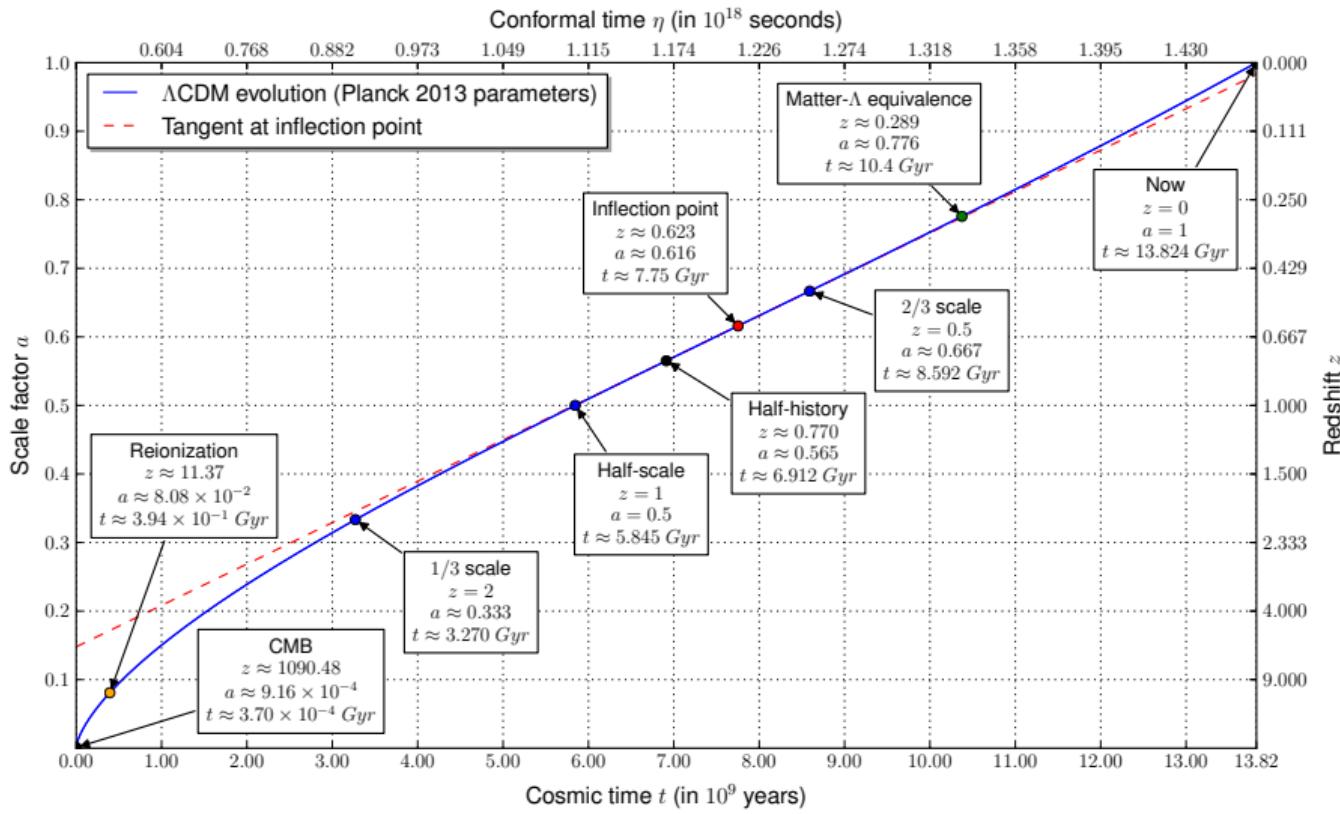
What did we just compute?

- The age of the Universe

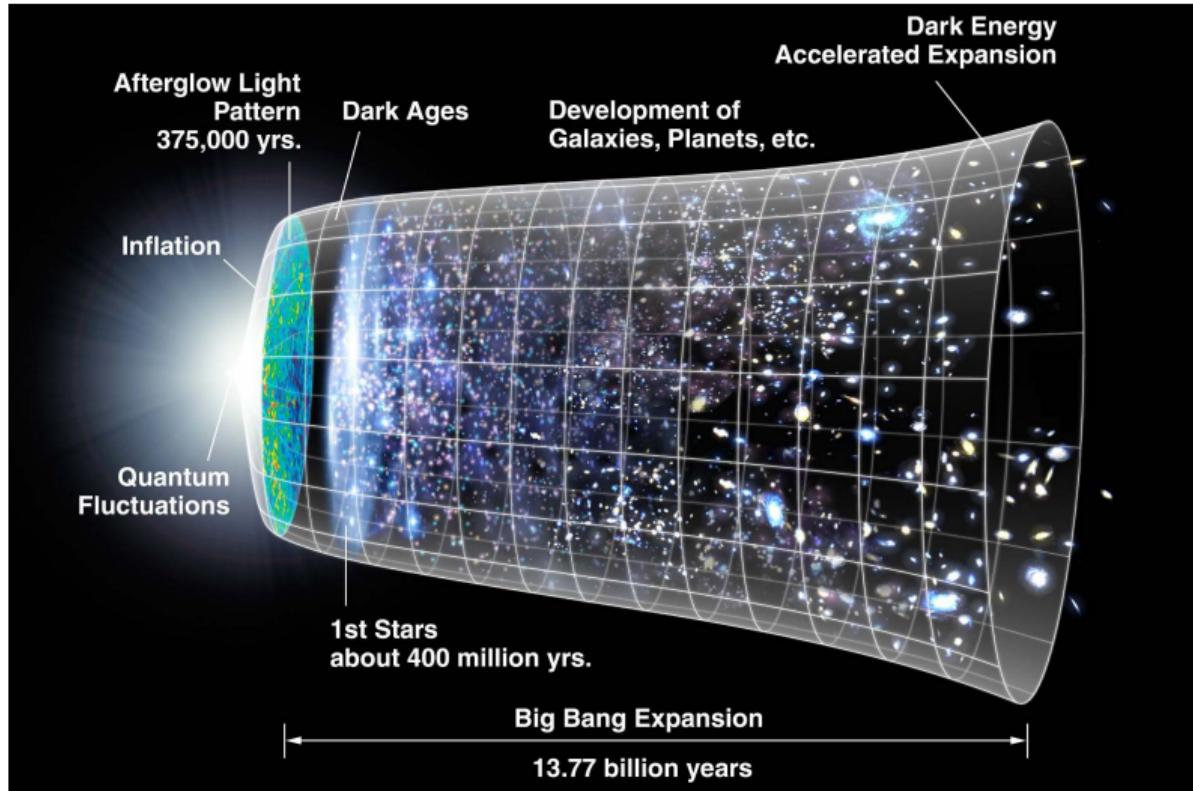
Conclusion

So we just computed the **Age of the Universe** in about **60 lines of C++20** !

Computing the evolution of the Universe



Our current understanding of the history of the Universe



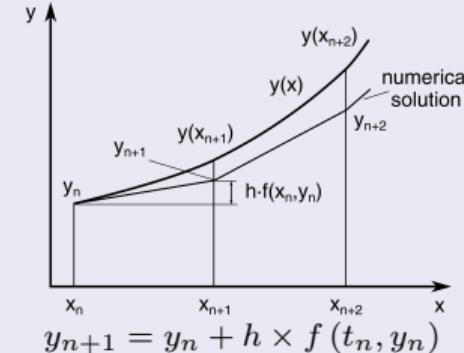
The solver

Coming back to the core of computation

```

1 // Function to integrate
2 auto da_dt = [&](auto t, auto a) {
3     return a * hubble_0 * std::sqrt(
4         omega_r0 * std::pow(a, static_cast<T>(-4))
5         + omega_m0 * std::pow(a, static_cast<T>(-3))
6         + omega_k0 * std::pow(a, static_cast<T>(-2))
7         + omega_l0
8    );
9 };
10 // Computation
11 while (a > std::numeric_limits<T>::epsilon()) {
12     evolution.emplace_back(std::array<T, 2>{{t, a}});
13     a = a - h * da_dt(t, a);
14     t = t - h;
15 }
```

Euler's method



$$G_{\mu\nu} = \frac{8\pi G}{c^4} T_{\mu\nu} \Rightarrow H^2 = \left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{3}\rho - \frac{kc^2}{a^2}$$

$$\dot{H} + H^2 = \frac{\ddot{a}}{a} = -\frac{4\pi G}{3} \left(\rho + \frac{3P}{c^2}\right) \Rightarrow \frac{H^2}{H_0^2} = \Omega_{R_0} a^{-4} + \Omega_{M_0} a^{-3} + \Omega_{k_0} a^{-2} + \Omega_{\Lambda_0}$$

Components

- Ω_R : radiation
- Ω_M : matter
- Ω_k : curvature
- Ω_Λ : dark-energy

Friedmann-Lemaître equation that is being solved

$$\frac{da(t)}{dt} = a(t) H_0 \sqrt{\Omega_{R_0} a(t)^{-4} + \Omega_{M_0} a(t)^{-3} + \Omega_{k_0} a(t)^{-2} + \Omega_{\Lambda_0}}$$

Going beyond

End of story?

No!

Plenty of things can be improved

- This is the simplest possible integrator: can we do better and achieve more **accuracy** and **precision**?
- Can we **parallelize** the code?
- Can we use **more modern constructs**?
- Can we make it **more generic**?
- ...

Firsts steps

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Toward an improved version

Integration function (1/4)

```
// Integrate the Friedmann-Lemaitre(-Robertson-Walker) equations
template <
    typename T,
    class Container = std::vector<std::tuple<T, T>>
>
requires std::is_floating_point_v<T>
Container integrate_flrw(
    const T a_0,
    const T hubble_0,
    const T omega_r0,
    const T omega_m0,
    const T omega_l0,
    const T dt,
    const T dt_backup,
    const T t_backward,
    const T t_forward
)
{
    // Constants
    using value_type = T;
    using container_type = Container;
    constexpr value_type zero = 0;
    constexpr value_type one = 1;
    constexpr value_type two = 2;
    constexpr value_type three = 3;
    constexpr value_type six = 6;
    constexpr value_type w_r = one / three;
    constexpr value_type w_m = zero;
    constexpr value_type w_k = -one / three;
    constexpr value_type w_l = -one;
```

Toward an improved version

Integration function (2/4)

```
// Initialization
const value_type omega = omega_r0 + omega_m0 + omega_l0;
const value_type omega_k0 = one - omega;
container_type past(1, std::make_pair(zero, a_0));
container_type future(1, std::make_pair(zero, a_0));

// Expression of da/dt
auto da_dt = [&](const value_type a, const value_type sign) {
    return std::copysign(one, sign) * a * hubble_0 * std::sqrt(
        omega_r0 * std::pow(a, -three * (one + w_r))
        + omega_m0 * std::pow(a, -three * (one + w_m))
        + omega_k0 * std::pow(a, -three * (one + w_k))
        + omega_l0 * std::pow(a, -three * (one + w_l)))
    );
};

// Runge-kutta of order 4
auto rk4 = [&](const value_type a, const value_type sign) {
    const value_type k1 = da_dt(a, sign);
    const value_type a1 = a + dt / two * k1;
    const value_type k2 = da_dt(a1, sign);
    const value_type a2 = a + dt / two * k2;
    const value_type k3 = da_dt(a2, sign);
    const value_type a3 = a + dt * k3;
    const value_type k4 = da_dt(a3, sign);
    return a + dt / six * (k1 + k2 + k2 + k3 + k3 + k4);
};
```

Toward an improved version

Integration function (3/4)

```
auto loop = [&](container_type& c, const value_type sign, const value_type t_lim) {
    // Initialization
    value_type t_sign = std::copysign(one, sign); value_type t_back = std::get<0>(c.back());
    value_type t_old = t_back; value_type t_new = t_back; bool t_ok = std::abs(t_new) < std::abs(t_lim);
    value_type a_sign = std::copysign(one, sign); value_type a_back = std::get<1>(c.back());
    value_type a_old = a_back; value_type a_new = a_back; bool a_ok = a_new > zero && std::isnormal(a_new);
    value_type origin = std::get<0>(c.back());
    c.reserve(std::abs(t_back - t_lim) / dt_backup);
    // Integration loop
    for (std::size_t i = 0; t_ok && a_ok; ++i) {
        t_new = origin + i * t_sign * dt;
        a_new = rk4(a_old, t_sign);
        a_ok = !(std::isnan(a_new) && a_old > a_0);
        if (!a_ok && !std::signbit(a_sign * t_sign)) {
            a_sign = -a_sign;
            a_new = rk4(a_old, a_sign);
        }
        t_ok = std::abs(t_new) < std::abs(t_lim);
        a_ok = a_new > zero && std::isnormal(a_new);
        if (t_ok && a_ok) {
            t_old = t_new;
            a_old = a_new;
            if (!(std::abs(t_back - t_new) < dt_backup)) {
                t_back = t_new;
                a_back = a_new;
                c.emplace_back(t_back, a_back);
            }
        } else if (std::abs(t_old - t_back) > zero) {c.emplace_back(t_old, a_old);}
    }
};
```

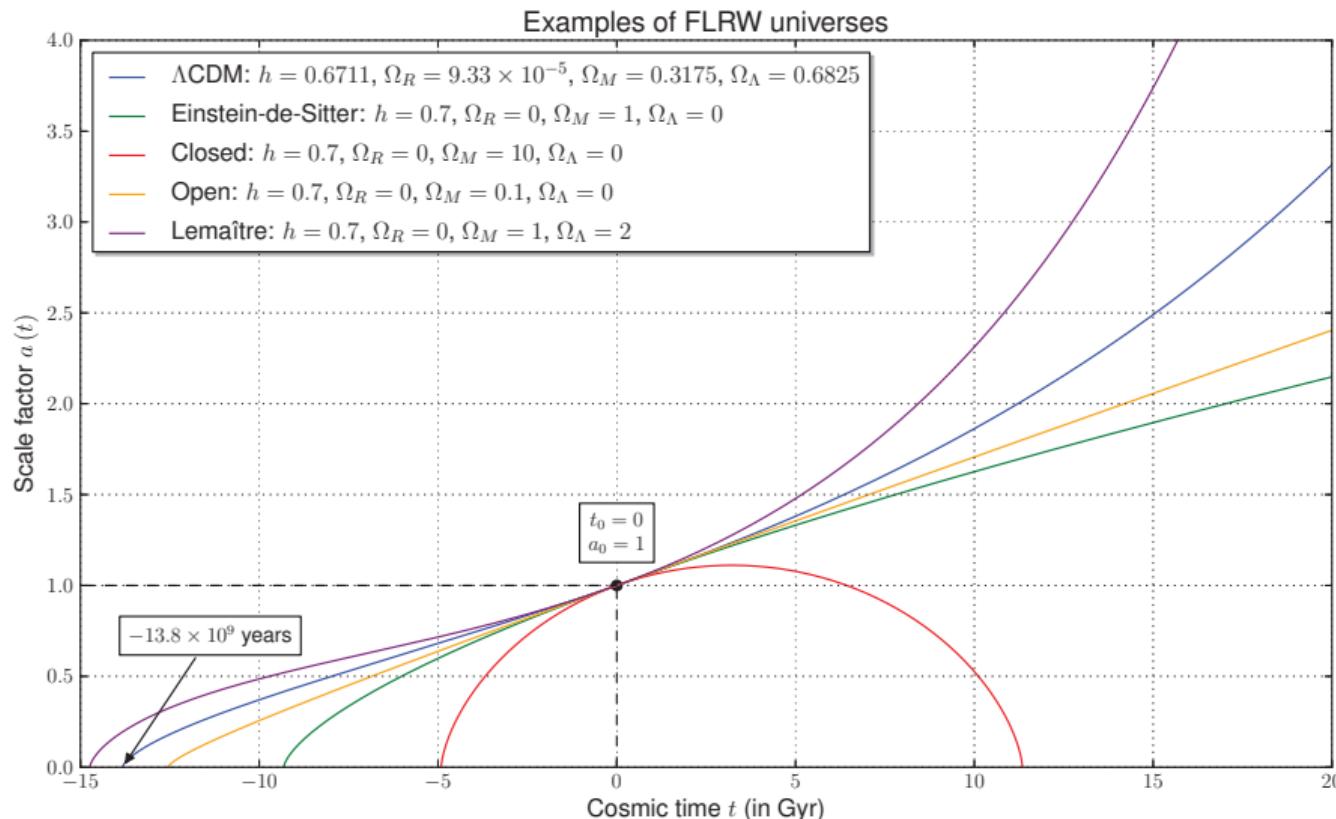
Toward an improved version

Integration function (4/4)

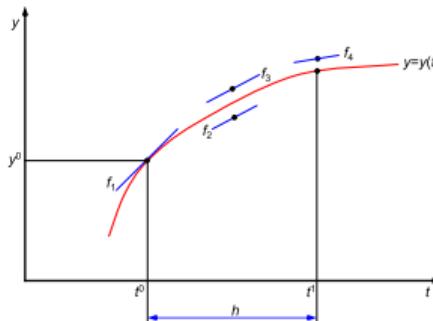
```
// Execution of backward and forward integration
std::thread backward(loop, std::ref(past), -one, t_backward);
std::thread forward(loop, std::ref(future), one, t_forward);

// Finalization
backward.join();
forward.join();
future.insert(future.begin(), past.rbegin(), past.rend()-1);
return future;
}
```

Toward an improved version



Runge-Kutta of order 4 (RK4)



Equations

$$k_1 = f(t_n, y_n)$$

$$k_2 = f\left(t_n + \frac{h}{2}, y_n + h \frac{k_1}{2}\right)$$

$$k_3 = f\left(t_n + \frac{h}{2}, y_n + h \frac{k_2}{2}\right)$$

$$k_4 = f(t_n + h, y_n + hk_3)$$

$$y_{n+1} = y_n + \frac{h}{6} (k_1 + 2k_2 + 2k_3 + k_4)$$

$$t_{n+1} = t_n + h$$

Code

```
// Runge-kutta of order 4
template <class T>
constexpr rk4(T t, T y, auto dy_dt, T dt) {
    // Step 1
    const T t1 = t;
    const T y1 = y;
    const T k1 = dy_dt(t1, y1);
    // Step 2
    const value_type t2 = t + dt / 2;
    const value_type y2 = y + dt / 2 * k1;
    const value_type k2 = dy_dt(t2, y2);
    // Step 3
    const value_type t3 = t + dt / 2;
    const value_type y3 = y + dt / 2 * k2;
    const value_type k3 = dy_dt(t3, y3);
    // Step 4
    const value_type t4 = t + dt;
    const value_type y4 = y + dt * k3;
    const value_type k4 = dy_dt(t4, y4);
    // Result
    return y + dt / 6 * (k1 + 2 * k2 + 2 * k3 + k4);
};
```

Sequentiality

- Every intermediate step k depends on the previous one!

Going multidimensionnal

Code

```
// Runge-kutta of order 4
template <class T, std::size_t N, class F>
requires std::floating_point<T> && std::invocable<F, T, std::array<T, N>>
constexpr std::array<T, N> rk4(T t, std::array<T, N> y, F dy_dt, T dt) {
    // Types and constants
    using value_type = T; using vector_type = std::array<T, N>;
    constexpr value_type two = 2; constexpr value_type six = 6;
    const value_type dt_2 = dt / two;
    // Variables
    value_type ti = t;
    vector_type yi;
    // Step 1
    ti = t;
    for (std::size_t j = 0; j < N; ++j) {yi[j] = y[j];}
    const vector_type k1 = dy_dt(ti, yi);
    // Step 2
    ti = t + dt_2;
    for (std::size_t j = 0; j < N; ++j) {yi[j] = y[j] + dt_2 * k1[j];}
    const vector_type k2 = dy_dt(ti, yi);
    // Step 3
    ti = t + dt_2;
    for (std::size_t j = 0; j < N; ++j) {yi[j] = y[j] + dt_2 * k2[j];}
    const vector_type k3 = dy_dt(ti, yi);
    // Step 4
    ti = t + dt;
    for (std::size_t j = 0; j < N; ++j) {yi[j] = y[j] + dt * k3[j];}
    const vector_type k4 = dy_dt(ti, yi);
    // Result
    for (std::size_t j = 0; j < N; ++j) {
        yi[j] = y[j] + dt / six * (k1[j] + two * k2[j] + two * k3[j] + k4[j]);
    }
    return yi;
};
```

Vector equation

$$Y(t_0) = Y_0$$

$$\frac{dY(t)}{dt} = f(t, Y)$$

Three-body problem equations

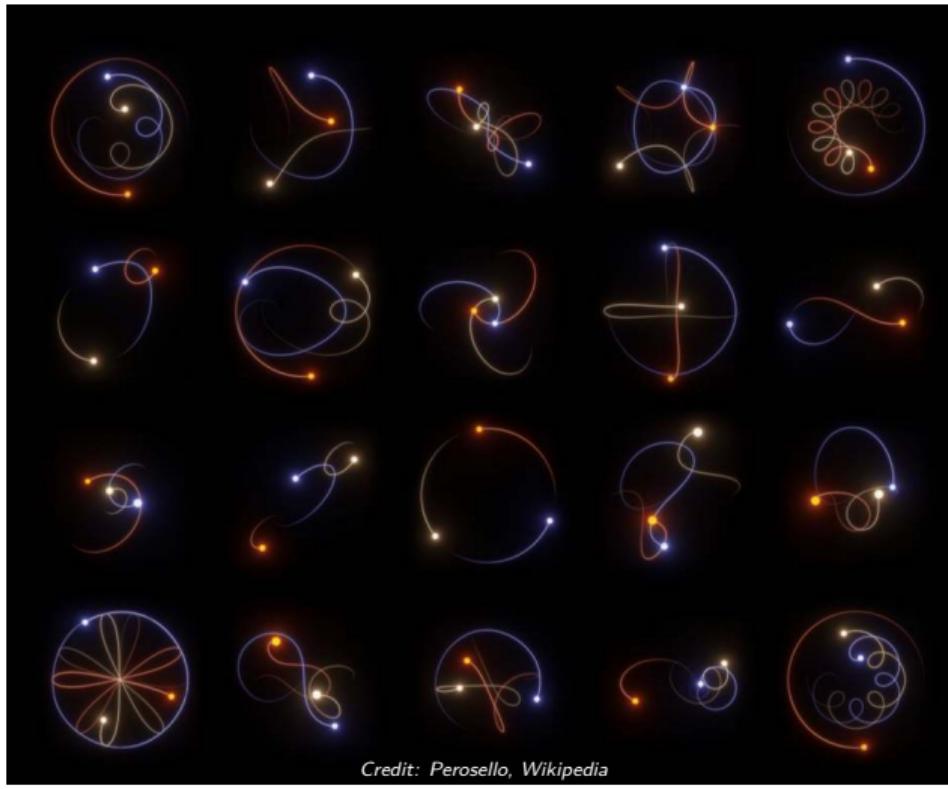
Code

```
// Three body problem
template <std::floating-point T>
constexpr std::array<T, 18> dy_dt(
    T t, std::array<T, 18> y,
    T G, T m1, T m2, T m3
) {
    constexpr std::size_t ndim = 3;
    std::array<T, 18> output = {};
    std::ranges::subrange x(std::begin(y) + 0, 9);
    std::ranges::subrange x1(std::begin(y) + 0, 3);
    std::ranges::subrange x2(std::begin(y) + 3, 3);
    std::ranges::subrange x3(std::begin(y) + 6, 3);
    const T d12 = std::hypot(x1[0] - x2[0], x1[1] - x2[1], x1[2] - x2[2]);
    const T d23 = std::hypot(x2[0] - x3[0], x2[1] - x3[1], x2[2] - x3[2]);
    const T d31 = std::hypot(x3[0] - x1[0], x3[1] - x1[1], x3[2] - x1[2]);
    std::ranges::subrange v(std::begin(y) + 9, 18);
    std::array<T, 3> a1 = {};
    std::array<T, 3> a2 = {};
    std::array<T, 3> a3 = {};
    for (std::size_t i = 0; i < ndim; ++i) {
        a1[i] = -G * m2 * (x1[i] - x2[i]) / std::pow(d12, 3)
            - G * m3 * (x1[i] - x3[i]) / std::pow(d31, 3);
        a2[i] = -G * m3 * (x2[i] - x3[i]) / std::pow(d23, 3)
            - G * m1 * (x2[i] - x1[i]) / std::pow(d12, 3);
        a3[i] = -G * m1 * (x3[i] - x1[i]) / std::pow(d31, 3)
            - G * m1 * (x3[i] - x2[i]) / std::pow(d23, 3);
    }
    std::copy(v, std::begin(output) + 0);
    std::copy(a1, std::begin(output) + 9);
    std::copy(a2, std::begin(output) + 12);
    std::copy(a3, std::begin(output) + 15);
    return output;
}
```

Vector equation

$$Y = \begin{pmatrix} x_1 \\ y_1 \\ z_1 \\ x_2 \\ y_2 \\ z_2 \\ x_3 \\ y_3 \\ z_3 \\ v_{x1} \\ v_{y1} \\ v_{z1} \\ v_{x2} \\ v_{y2} \\ v_{z2} \\ v_{x3} \\ v_{y3} \\ v_{z3} \end{pmatrix} \quad \frac{dY}{dt} = \begin{pmatrix} v_{x1} \\ v_{y1} \\ v_{z1} \\ v_{x2} \\ v_{y2} \\ v_{z2} \\ v_{x3} \\ v_{y3} \\ v_{z3} \\ a_{x1} \\ a_{y1} \\ a_{z1} \\ a_{x2} \\ a_{y2} \\ a_{z2} \\ a_{x3} \\ a_{y3} \\ a_{z3} \end{pmatrix}$$

Three-body problem visualizations



Problems

To achieve long-term correct integration, far better integrators are needed.

Going beyond

After this gentle introduction, we will dive into the details!

Context

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2 Firsts steps

3 Context

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An ambiguity

Integrals

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

- *Numerical integration* as in the computation of the numerical value of a **definite integral**
- Synonyms: **quadrature**, sometimes cubature in higher-dimensions ($\int \int$, $\int \int \int$, ...)

Differential equations

$$\frac{dy}{dt} = f(t, y(t)) \quad y(t_0) = y_0$$

$$f : [t_0, +\infty) \times \mathbb{R}^d \rightarrow \mathbb{R}^d \quad y_0 \in \mathbb{R}^d$$

- *Numerical integration* as in numerical methods for **Ordinary Differential Equations** (ODEs)
- Synonym: **differential equation solver**
- The term integration can go beyond ODEs, and include many other types of differential equations

Definite integrals and differential equations

An equivalence

$$\int f(x) dx \Leftrightarrow \frac{dy}{dx} = f(x)$$

- Finding antiderivatives \Leftrightarrow solving an ODE

Algorithms for definite integrals

- Gaussian quadrature
- Clenshaw-Curtis quadrature
- Romberg's method
- ...

Algorithms for ordinary differential equations

- Euler's method
- Runge-Kutta methods (RK)
- General Linear Methods (GLM)
- ...

This talk (because we only have 1h!)

- Focus on **Ordinary Differential Equations**
- *Integrators mean differential equations solvers*

The lands of differential equations



Differential equation solvers

- In reality go way beyond this map
- Including Partial Differential Equations (PDEs)

This talk

- Focus on good old classical
Ordinary Differential Equations

Going beyond

- Many techniques presented here
can be extended to other types of
solvers

In programming languages



Python

- `scipy.integrate`

Julia

- `DifferentialEquations.jl`

C++

- `Boost.Numeric.Odeint`

Comparison with C++

- `Boost.Numeric.Odeint`: Copyright 2009-2015 Karsten Ahnert and Mario Mulansky
- C++ is stuck in the past, other languages do far better in terms of everything: functionality, ease of use, and even performance

This talk

- The goal **is NOT** to revolutionize everything or show a library that beats everything
- The goal **is** to start from the foundation and illustrate a path forward with basic examples

Theoretical foundations

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Problem statement: Initial Value Problem (IVP)

Ordinary Differential Equation (ODE)

$$\frac{dy(t)}{dt} = f(t, y(t))$$
$$f : [t_0, +\infty) \times \mathbb{R}^d \rightarrow \mathbb{R}^d$$

Initial condition

$$y(t_0) = y_0$$
$$y_0 \in \mathbb{R}^d$$

Mathematical and software architecture

Question

- How to abstract the problem?

Mathematical abstractions

- Well-posed and abstracted in mathematics ⇒ “easy” to abstract in software
- Mathematical architecture ⇒ Software architecture

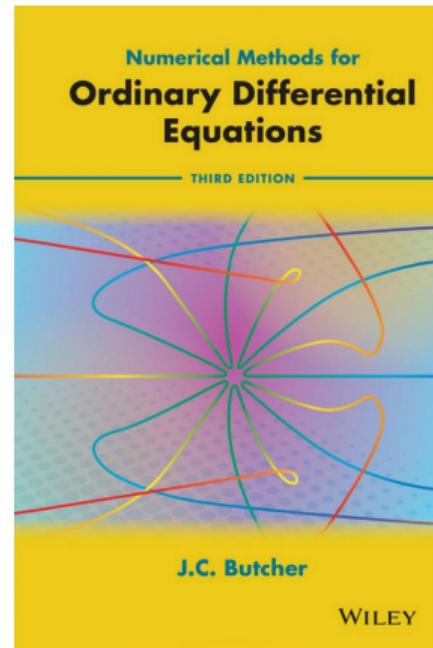
Counter-example: units

- Intuitively understood in physics
- But very fuzzy foundations in mathematics
- ⇒ Incredibly hard to abstract correctly in software

The mathematical architecture of algorithms



John C. Butcher



Numerical Methods for Ordinary Differential Equations, Third Edition
John C. Butcher
John Wiley & Sons, 2016

Main classes of algorithms

Runge-Kutta Methods (RK)

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i k_i \quad k_i = f(t_n + c_i h, y_n + (a_{i1}k_1 + a_{i2}k_2 + \dots + a_{i,i-1}k_{i-1})h)$$

Linear Multistep Methods (LLM)

$$\begin{aligned} y_{n+s} + a_{s-1} \cdot y_{n+s-1} + a_{s-2} \cdot y_{n+s-2} + \dots + a_0 \cdot y_n &= h \cdot \left(b_s \cdot f(t_{n+s}, y_{n+s}) + \dots + b_0 \cdot f(t_n, y_n) \right) \\ \Leftrightarrow \sum_{j=0}^s a_j y_{n+j} &= h \sum_{j=0}^s b_j f(t_{n+j}, y_{n+j}) \end{aligned}$$

General Linear Methods (GLM)

$$y^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix}, \quad y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix}, \quad Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_s \end{bmatrix}, \quad F = \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_s \end{bmatrix} = \begin{bmatrix} f(Y_1) \\ f(Y_2) \\ \vdots \\ f(Y_s) \end{bmatrix}$$

$$Y_i = \sum_{j=1}^s a_{ij} h F_j + \sum_{j=1}^r u_{ij} y_j^{[n-1]}, \quad i = 1, 2, \dots, s \quad y_i^{[n]} = \sum_{j=1}^s b_{ij} h F_j + \sum_{j=1}^r v_{ij} y_j^{[n-1]}, \quad i = 1, 2, \dots, r$$

Different approaches

Runge-Kutta Methods (RK)

- May use intermediary steps
- But discard the information
- Only need

Linear Multistep Methods (LMM)

- Take advantages of previous steps to improve efficiency

General Linear Methods (GLM)

- Can combine advantages of both approaches

Explicit methods

- Solution at the next time step is computed directly using only the information from previous steps
- **Less robust for stiff problems**

Implicit methods

- Solution implicitly defined through an equation that includes the unknown future value
- A system of equations need to be solved at each time step
- **Better stability for stiff problems**

Mathematical abstraction

Butcher tableau for Runge-Kutta methods (explicit)

c_1	$a_{1,1}$	0	0	...	0	0
c_2	$a_{2,1}$	$a_{2,2}$	0	...	0	0
c_3	$a_{3,1}$	$a_{3,2}$	$a_{3,3}$...	0	0
c	A	⋮	⋮	⋮	⋮	⋮
b^T	⋮	⋮	⋮	⋮	⋮	⋮
c_{s-1}	$a_{s-1,1}$	$a_{s-1,2}$	$a_{s-1,3}$...	$a_{s-1,s-1}$	0
c_s	$a_{s,1}$	$a_{s,2}$	$a_{s,3}$...	$a_{s,s-1}$	$a_{s,s}$
	b_1	b_2	b_3	...	b_{s-1}	b_s

- $a_{i,j}$: **coefficients** (A : Runge-Kutta matrix)
- b_j : **weights**
- c_i : **nodes**
- s : number of **stages**

Design of methods

- The coefficients, weights, nodes have to be carefully derived and will determine the properties of the corresponding method

Adaptive Runge-Kutta methods

Butcher tableau for explicit adaptive Runge-Kutta methods

c_1	$a_{1,1}$	0	0	\dots	0	0
c_2	$a_{2,1}$	$a_{2,2}$	0	\dots	0	0
c_3	$a_{3,1}$	$a_{3,2}$	$a_{3,3}$	\dots	0	0
c	A					
b^T	\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
\tilde{b}^T	c_{s-1}	$a_{s-1,1}$	$a_{s-1,2}$	$a_{s-1,3}$	\dots	$a_{s-1,s-1}$
	c_s	$a_{s,1}$	$a_{s,2}$	$a_{s,3}$	\dots	$a_{s,s-1}$
		b_1	b_2	b_3	\dots	b_{s-1}
		\tilde{b}_1	\tilde{b}_2	\tilde{b}_3	\dots	\tilde{b}_{s-1}
						b_s
						\tilde{b}_s

$$\tilde{y}_{n+1} = y_n + h \sum_{i=1}^s \tilde{b}_i k_i$$

$$e_{n+1} = \tilde{y}_{n+1} - y_{n+1} = h \sum_{i=1}^s (\tilde{b}_i - b_i) k_i \quad (\text{error estimate})$$

Implicit Runge-Kutta methods

Butcher tableau for implicit adaptive Runge-Kutta methods

c_1	$a_{1,1}$	$a_{1,2}$	$a_{1,3}$	\dots	$a_{1,s-1}$	$a_{1,s}$
c_2	$a_{2,1}$	$a_{2,2}$	$a_{2,3}$	\dots	$a_{2,s-1}$	$a_{2,s}$
c_3	$a_{3,1}$	$a_{3,2}$	$a_{3,3}$	\dots	$a_{3,s-1}$	$a_{3,s}$
c	A					
b^T	\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
\tilde{b}^T	c_{s-1}	$a_{s-1,1}$	$a_{s-1,2}$	$a_{s-1,3}$	\dots	$a_{s-1,s-1}$
	c_s	$a_{s,1}$	$a_{s,2}$	$a_{s,3}$	\dots	$a_{s,s-1}$
		b_1	b_2	b_3	\dots	b_{s-1}
		\tilde{b}_1	\tilde{b}_2	\tilde{b}_3	\dots	\tilde{b}_{s-1}
						b_s
						\tilde{b}_s

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i k_i$$

$$k_i = f \left(t_n + c_i h, y_n + h \sum_{j=1}^s a_{ij} k_j \right), \quad i = 1, \dots, s$$

Linear Multistep Methods (LMM)

Specification

$$\begin{aligned}y_n = & \alpha_1 y_{n-1} + \alpha_2 y_{n-2} + \cdots + \alpha_k y_{n-k} \\& + \beta_0 h f(x_n, y_n) + \beta_1 h f(x_{n-1}, y_{n-1}) + \cdots + \beta_k h f(x_{n-k}, y_{n-k})\end{aligned}$$

The method is specified by $[\alpha, \beta]$ where:

$$\begin{aligned}\alpha(z) &= 1 - \alpha_1 z - \alpha_2 z^2 - \cdots - \alpha_k z^k \\ \beta(z) &= \beta_0 + \beta_1 z + \beta_2 z^2 + \cdots + \beta_k z^k\end{aligned}$$

General Linear Methods (GLM)

General abstraction

$$\begin{bmatrix} A & U \\ B & V \end{bmatrix}$$

with

A of size $s \times s$

B of size $r \times s$

U of size $s \times r$

V of size $r \times r$

$$Y_i = \sum_{j=1}^s a_{ij} h F_j + \sum_{j=1}^r u_{ij} y_j^{[n-1]}, \quad i = 1, 2, \dots, s$$

$$y_i^{[n]} = \sum_{j=1}^s b_{ij} h F_j + \sum_{j=1}^r v_{ij} y_j^{[n-1]}, \quad i = 1, 2, \dots, r$$

$$\Rightarrow \begin{bmatrix} Y \\ y^{[n]} \end{bmatrix} = \begin{bmatrix} A & U \\ B & V \end{bmatrix} \begin{bmatrix} hF \\ y^{[n-1]} \end{bmatrix}$$

Relationships between RKs, LMMs, and GLMs

- Runge-Kutta and Linear Multisteps methods can be represented through $\begin{bmatrix} A & U \\ B & V \end{bmatrix}$
- They can be seen as special cases of General Linear Methods

Special cases of the general framework

Runge-Kutta

- Euler
- Heun's method
- Runge-Kutta-Fehlberg method
- Cash-Karp method
- Dormand-Prince method
- Runge-Kutta-Nystrom methods
- Crank-Nicolson method
- Gauss-Legendre methods
- Lobatto methods
- Radau methods
- ...

Linear Multistep Methods

- Backward Differentiation Formulas
- Adams-Basforth methods
- Adams-Moulton methods
- ...

General Linear Methods

- Diagonally Implicit Multistage Integration Methods
- Almost Runge-Kutta methods
- G-symplectic methods
- ...

Strategy

- Use the General Linear Methods matrix A, U, B, V as a foundation for the software architecture

Outline of an implementation

1 Introduction

2 Firsts steps

3 Context

4 Theoretical foundations

5 Outline of an implementation

6 Conclusion

Implementation strategy

This talk

- This talk: we will focus on Runge-Kutta subcase using Butcher's tableau a_{ij}, b_j, c_i
- Generalizing to GLM would use the same approach

Reminder

c	c_1	$a_{1,1}$	$a_{1,2}$	$a_{1,3}$	\dots	$a_{1,s-1}$	$a_{1,s}$
	c_2	$a_{2,1}$	$a_{2,2}$	$a_{2,3}$	\dots	$a_{2,s-1}$	$a_{2,s}$
	c_3	$a_{3,1}$	$a_{3,2}$	$a_{3,3}$	\dots	$a_{3,s-1}$	$a_{3,s}$
b^T	\vdots	\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
\tilde{b}^T	c_{s-1}	$a_{s-1,1}$	$a_{s-1,2}$	$a_{s-1,3}$	\dots	$a_{s-1,s-1}$	$a_{s-1,s}$
	c_s	$a_{s,1}$	$a_{s,2}$	$a_{s,3}$	\dots	$a_{s,s-1}$	$a_{s,s}$
		b_1	b_2	b_3	\dots	b_{s-1}	b_s
		\tilde{b}_1	\tilde{b}_2	\tilde{b}_3	\dots	\tilde{b}_{s-1}	\tilde{b}_s

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i k_i \quad k_i = f \left(t_n + c_i h, y_n + h \sum_{j=1}^s a_{ij} k_j \right), \quad i = 1, \dots, s$$

Target

This talk

- We'll have Verner's most efficient Runge-Kutta pairs in mind: <https://www.sfu.ca/jverner/>

Adaptive Runge-Kutta pairs with interpolants

- Runge-Kutta (7)6 Pair with Interpolants (July 2024)
- Runge-Kutta (8)7 Pair with Interpolants (May 2024)
- Runge-Kutta (9)8 Pair with Interpolants (April 2024)

Verner's methods

- Explicit adaptive Runge-Kutta schemes
- Slightly enhanced methods with interpolants
- High-accuracy interpolation inside integration steps

Interpolation with extra coefficients β_i

$$y_{n+u} = y_n + h \sum_{i=1}^{s^*} \beta_i(u) F_i \quad \text{at} \quad x_n + uh, \quad u \in [0, 1]$$

See *Numerically optimal Runge-Kutta pairs with interpolants*, J.H. Verner, Springer Science, 2009

Verner's coefficients examples

```
#####
# MODES
#
# A better 'efficient' Runge-Kutta (16:8,9) pair
#
These are approximate REAL coefficients computed
using MAPLE with 40 digits for
#
a slightly more efficient SIXTEEN-stage conventional
pair of methods of orders p=8 and p=9, with
dominant stage order = 9.
#
Together with approximate 40-digit coefficients
for two interpolants of orders 8 and 9 that
require 5 and 6 extra stages, respectively.
#
Exact coefficients of the method are possible using
surd in terms of sqrt(6). Exact coefficients for the
method are possible using surds in terms of
cubic polynomial that are surds in
terms of sqrt(6). Hence, exact coefficients for the
interpolants cannot be conveniently represented.
#
This procedure is a better efficient pair in the
sense that for an unrestricted maximum coefficient
from b and A, it has a propagating formula with
a minimum 2-norm of the local truncation error as
as follows:
#
T_16,2 = -.00000854399
#
This 2-norm is slightly smaller than T16,2 for the
(16:9,9) pair tabulated above. This 2-norm has two
local maximum values on [0,1].
#
Additional stages and interpolating weights allow
for the computation of an approximation of order up
to order 16. They are described below. These
interpolants have continuous derivatives.
#
Nodes c[17]=1, c[18] = c[19] were selected to
minimize the maximum of the 2-norms of the local
truncation error over the interval [0,1] for the
interpolant of order 8, and this value is
T_8,2 = -.000008721
#
This 2-norm has three local maximum values on [0,1].
#
The remaining five nodes were selected in an attempt
to minimize the maximum of the 2-norms of the local
truncation error over the interval [0,1] for the
interpolant of order 9, and this value is
T_16,2 = -.000008789
#
This 2-norm has two local maximum values on [0,1].
#
The formulas scanned for this optimal formula are
those developed in J.H. Verner, SIAM J. NA 1978, 772-798,
"Explicit Runge-Kutta methods with estimates of the
Local Truncation Error". It is conceivable that the
pairs found in that paper are also optimal. See also
Verner, J.H., "A Family of High Order Explicit Runge-Kutta
Pairs with Low Stage Order", which also require 16 stages,
but are not necessarily optimal. In fact, they may
yield particular pairs of equivalent or more
efficiency. Coefficients for the interpolants are
those developed in J.H. Verner, SIAM J. NA 1993,
104, 345-357, "Differentiable Interpolants for High order
Runge-Kutta methods".
#
Instructions for using the interpolants are contained
in J.H. Verner, SIAM J. NA 1993, 1446-1466, "Differentiable
Interpolants for high-order Runge-Kutta methods".
#
#####

```

```
#####
# MODES
#
# c[1] = 0
# c[2] = .3571e-1
# c[3] = -.998602899126741497286229954998445721428e-1
# c[4] = -.1555942136911211089334358234856085213
# c[5] = .6358
# c[6] = .2327359473638652675663168928903288192566
# c[7] = .553864852039437324336819710989711807434
# c[8] = .18069683208089880875617860
# c[9] = .491625
# c[10] = .8658e-1
# c[11] = .05206417954120494478822880880875617860
# c[12] = .8389
# c[13] = .8900
# c[14] = .1
# c[15] = .1
# c[16] = 1
#
#####
# COUPLING COEFFICIENTS
#
#####
# for c[11] = 0
#
# for c[2] = .3571e-1
#
# for c[3] = -.998602899126741497286229954998445721428e-1
# a[3,11] = -.383137556971037625757228897924291143273e-1
# a[3,21] = .1373970372944730957582871137575
# for c[4] = .145958421369811211089334358234856085213
# a[4,11] = .37147605342252892792338959871417145532e-1
# a[4,21] = 0
# a[4,31] = .3114420146206750846318097606761425143669
# for c[5] = .176764240871505111918434780668033362
# a[5,11] = .4627764240871505111918434780668033362
# a[5,21] = 0
# a[5,31] = -.982302134885293641180195135423594
# a[5,41] = .7221877501378172472466864586228145
# for c[6] = .2327359473638652675663168928903288192566
# a[6,11] = .524210858577351689841491119318449756747e-1
# a[6,21] = 0
# a[6,31] = 0
# a[6,41] = .17969111959366127948669977364298984
# a[6,51] = .623787937193856336807351972187917439276e-3
# for c[7] = .553864852039437324336819710989711087434
# a[7,11] = .159245223284763206399159129732726793
# a[7,21] = 0
# a[7,31] = 0
# a[7,41] = -.42984298772410757081891856646998803751595
# a[7,51] = .46605265427280808512454596239448211072e-1
# a[7,61] = .7578051327121986337219863351834241158
#
# for c[8] = .8555
# a[8,11] = .228333333333333333333333333333333333333e-1
# a[8,21] = 0
# a[8,31] = 0
# a[8,41] = 0
# a[8,51] = 0
# a[8,61] = .3359345986651036797134211956931057628
# a[8,71] = .24673220760915630795324452750935690048
# for c[9] = .491625
# a[9,11] = .72975585973e-1
# a[9,21] = 0
# a[9,31] = 0
# a[9,41] = 0
# a[9,51] = 0
# a[9,61] = .3348869729989333321298455323262028893
# a[9,71] = -.11841523951666466871951644675671318197
# a[9,81] = -.34857382125e-1
#
```

```
#####
# for c[10] = .6858e-1
# a[10,11] = .4911213663452096382929799914888692571185e-1
# a[10,21] = 0
# a[10,31] = 0
# a[10,41] = 0
# a[10,51] = 0
# a[10,61] = .39838573613895234709880841295495424467e-1
# a[10,71] = .108967529899358412077394761365105244466
# a[10,81] = -.21742591534584779845568958976229518988e-1
# a[10,91] = -.1859564746936462523123330439517694660
#
# for c[11] = .253
# a[11,11] = .2767948618641218048917506286477493636734e-1
# a[11,21] = 0
# a[11,31] = 0
# a[11,41] = 0
# a[11,51] = 0
# a[11,61] = .333e-1
# a[11,71] = -.145452607863945875562704851519709898651
# a[11,81] = .24793332209524424293265797085546567159e-1
# a[11,91] = .13852948944399210486539921215879453749
# a[11,101] = .2185234256411259838011127284294639672873
#
# for c[12] = .6612041795128459447892126848966897617864
# a[12,11] = .55846577091698827725262810862204488941540e-1
# a[12,21] = 0
# a[12,31] = 0
# a[12,41] = 0
# a[12,51] = 0
# a[12,61] = -.9400211008723188074795478993131131059e-1
# a[12,71] = .2325399655282794595188121105827
# a[12,81] = .102384122489748798316672186561113729e-1
# a[12,91] = -.24793332209524424293265797085546567159e-2
# a[12,101] = .145452607863945875562704851519709898651
# a[12,111] = .255976470769604185584747469949588614607
#
# for c[13] = .8389
# a[13,11] = .4802310512723159893183945790088387738204
# a[13,21] = 0
# a[13,31] = 0
# a[13,41] = 0
# a[13,51] = 0
# a[13,61] = -.3561041025355999191669726128737898100
# a[13,71] = .187133089884813851866958933836802086700
# a[13,81] = .546876663357946674793146073318438308509124
# a[13,91] = .573476587784095687599871981692639407295
# a[13,101] = .13472599468130497736173946644609357523
# a[13,111] = .590462453352472833173399656466856456499
# a[13,121] = .6590462453352472833173399656466856456499
#
# for c[14] = .9886
# a[14,11] = .23873320874714410789759842476283805310009
# a[14,21] = 0
# a[14,31] = 0
# a[14,41] = 0
# a[14,51] = 0
# a[14,61] = 5-.9562917088298331195843181398154563177
# a[14,71] = .144285520877119361866837782531987432410
# a[14,81] = .741025232144207177852540966672054728101
# a[14,91] = -.71181929345795111338466526473999638
# a[14,101] = .5-.9400211008723188074795478993131131059e-1
# a[14,111] = .14848027254470895330886727384877043098
# a[14,121] = .24831972319838615758965611386333981843
#
# for c[15] = 1
# a[15,11] = .584711122988441895171986080772221315
# a[15,21] = 0
# a[15,31] = 0
# a[15,41] = 0
# a[15,51] = 0
# a[15,61] = -.124186017112673046214666699108813084670
# a[15,71] = .348454545454893184697798341211309120189
# a[15,81] = -.2242610531116623298599912513730431746999
# a[15,91] = -.8828857053805458252698999251378431476999
# a[15,101] = 1.37H1512853879848641386473734748434464
```

Example: A better efficient Runge-Kutta (16:8,9) pair on Verner's website



Architecture

A Runge-Kutta method can be abstracted by:

- a_{ij} : Runge-Kutta coefficients \Rightarrow 2D array
- b_j^n : weights \Rightarrow a sequence of 1D arrays (1 for non-adaptive, generally 2 for adaptive)
- c_i : nodes \Rightarrow a sequence of 1D array
- β_j^n : interpolants: \Rightarrow a sequence of 1D arrays (one for each b^n)

General idea

```
using rk = make_runge_kutta<  
    runge_kutta_coefficients,  
    runge_kutta_weights,  
    runge_kutta_nodes,  
    runge_kutta_interpolants,  
    ...  
>;
```

Approach

Recursive generation

We want to generate the following automatically from the coefficients:

$$\begin{aligned}y_{n+1} &= y_n + h \sum_{i=1}^s b_i k_i \\k_i &= f \left(t_n + c_i h, y_n + h \sum_{j=1}^s a_{ij} k_j \right), \quad i = 1, \dots, s\end{aligned}$$

Performance concerns

- The Butcher Tableau can be very sparse
- Null coefficients should be optimized away
- Compilers may not be able to do it because of floating-point special values

Meta-programming helpers

What we want to be able to type

```
using runge_kutta_coefficients = make_coefficient_array<
    indexer[0, 0] = coefficient<double>(/*value*/),
    indexer[1, 0] = coefficient<double>(/*value*/),
    indexer[1, 1] = coefficient<double>(/*value*/),
    indexer[2, 0] = coefficient<double>(/*value*/),
    //...
>;
```

Indexing strategy

```
// Generic case to build an AST
template <class... Ts>
struct indexer_type {
    // Constructor
    constexpr indexer_type(Ts... i): indices(i...) {}
    // Build an AST
    template <class T>
    constexpr indexer_expression<index_type, coefficient<double>> operator=(coefficient<double> c) {
        return indexer_expression(*this, c);
    }
    // Indices
    const std::tuple<Ts...> indices;
};
// Specialization
template <>
struct indexer_type<void> {
    template <class... Args>
    constexpr indexer_type<Args...> operator[](Args... args) const noexcept {return indexer_type(args...);}
};
// Builder to be able to type indexer[i, j]
inline constexpr indexer_type<void> indexer;
```

Meta-programming helpers

Transformation

```
using runge_kutta_coefficients = make_coefficient_array<
    indexer[0, 0] = coefficient<double>(/*value*/),
    indexer[1, 0] = coefficient<double>(/*value*/),
    indexer[1, 1] = coefficient<double>(/*value*/),
    indexer[2, 0] = coefficient<double>(/*value*/),
    //...
>;
```

will compile-into:

```
using runge_kutta_coefficients = make_coefficient_array<
    indexer_expression<indexer<std::size_t, std::size_t>, coefficient<double>>,
    indexer_expression<indexer<std::size_t, std::size_t>, coefficient<double>>,
    indexer_expression<indexer<std::size_t, std::size_t>, coefficient<double>>,
    indexer_expression<indexer<std::size_t, std::size_t>, coefficient<double>>,
    //...
>;
```

Details

See the talk of last year for the implementation of this kind of expression templates:
Symbolic Calculus for High-Performance Computing from Scratch using C++23, V. Reverdy, CppCon2023

Sorting

Array of expressions

```
using runge_kutta_coefficients = make_coefficient_array<
    indexer_expression<indexer<std::size_t, std::size_t>, coefficient<double>>,
    indexer_expression<indexer<std::size_t, std::size_t>, coefficient<double>>,
    indexer_expression<indexer<std::size_t, std::size_t>, coefficient<double>>,
    // ...
>;
```

Unique order

```
using runge_kutta_coefficients = make_coefficient_array<
    indexer[0, 0] = coefficient<double>(/*value*/),
    indexer[1, 0] = coefficient<double>(/*value*/),
    // ...
>;
```

and

```
using runge_kutta_coefficients = make_coefficient_array<
    indexer[1, 0] = coefficient<double>(/*value*/),
    indexer[0, 0] = coefficient<double>(/*value*/),
    // ...
>;
```

need to collapse to the same type!

C++26 proposal that will help

- Language constructs to uniquely order types
- See P2830R4: Standardized Constexpr Type Ordering, G. Azman & N. Nichols

Indexing strategy

Strategy outline

- indexer_expression will generate an indexed_coefficient
- indexed_coefficient will have an access operator that will return a numeric_constant
- numeric_constant will hijack the compiler's arithmetic

Indexed coefficient outline

```
template <class Index, class Coefficient>
struct indexed_coefficient {
    using index_type = Index;
    using coefficient_type = Coefficient;
    using value_type = coefficient_type::value_type;
    static constexpr index_type index = {};
    static constexpr coefficient_type coefficient = {};
    constexpr value_type operator()(index_type) const noexcept {
        return coefficient_type::value;
    }
    constexpr coefficient_type operator[](index_type) const noexcept {
        return {};
    }
};
```

Accessing via overload resolution

indexed_coefficient_sequence[index<1, 2>] will redirect with the correct indexed_coefficient

Highjacking arithmetic (1/3)

Numeric constant

```
template <class T, T v>
requires std::is_arithmetic_v<T>
struct numeric_constant {
    using value_type = T;
    using type = numeric_constant<T, v>;
    static constexpr T value = v;
    constexpr operator value_type() const noexcept {
        return v;
    }
    template <class U>
    requires std::is_arithmetic_v<U>
    explicit constexpr operator U() const noexcept {
        return v;
    }
    constexpr value_type operator()() const noexcept {
        return v;
    }
};

template <class T, auto v>
requires std::is_arithmetic_v<T> && std::is_arithmetic_v<decltype(v)>
constexpr numeric_constant<T, static_cast<T>(v)> make_numeric_constant(
) noexcept {
    return {};
}
```

Highjacking arithmetic (2/3)

Null constant

```
template <class T>
using null_constant = numeric_constant<T, static_cast<T>(0)>;
```

```
template <class T>
struct is_null_constant: std::false_type {};
```

```
template <class T, T v>
struct is_null_constant<numeric_constant<T, v>>:
std::bool_constant<v == static_cast<T>(0)> {};
```

```
template <std::floating_point T, T v>
struct is_null_constant<numeric_constant<T, v>>:
std::bool_constant<
    std::isfinite(v) &&
    !(std::isless(v, static_cast<T>(0)) || std::isgreater(v, static_cast<T>(0)))
> {};
```

```
template <class T>
constexpr bool is_null_constant_v = is_null_constant<T>::value;
```

```
template <class T>
requires std::is_arithmetic_v<T>
constexpr null_constant<T> make_null_constant() noexcept {
    return {};
}
```

Highjacking arithmetic (3/3)

Operators

```
template <class T1, T1 v1, class T2, T2 v2>
requires (!is_null_constant_v<numeric_constant<T1, v1>>) && (!is_null_constant_v<numeric_constant<T2, v2>>)
constexpr numeric_constant<std::common_type_t<T1, T2>, v1 + v2>
operator+(numeric_constant<T1, v1>, numeric_constant<T2, v2>) noexcept {return {};}

template <class T1, T1 v1, class T2>
requires (!is_null_constant_v<numeric_constant<T1, v1>>) && is_null_constant_v<null_constant<T2>>
constexpr numeric_constant<std::common_type_t<T1, T2>, v1>
operator+(numeric_constant<T1, v1>, null_constant<T2>) noexcept {return {};}

template <class T1, class T2, T2 v2>
requires is_null_constant_v<null_constant<T1>> && (!is_null_constant_v<numeric_constant<T2, v2>>)
constexpr numeric_constant<std::common_type_t<T1, T2>, v2>
operator+(null_constant<T1>, numeric_constant<T2, v2>) noexcept {return {};}

template <class T1, class T2>
requires is_null_constant_v<null_constant<T1>> && is_null_constant_v<null_constant<T2>>
constexpr null_constant<std::common_type_t<T1, T2>>
operator+(null_constant<T1>, null_constant<T2>) noexcept {return {};}

template <class T1, T1 v1, class T2>
requires (!is_null_constant_v<numeric_constant<T1, v1>>) && std::is_arithmetic_v<T2>
constexpr std::common_type_t<T1, T2>
operator+(numeric_constant<T1, v1>, T2 v2) noexcept {return v1 + v2;}

// etc...
```

New rules

Rewriting arithmetic rules

- `numeric_constant<T, v>{} + numeric_constant<T, 0>{}` collapses to `numeric_constant<T, v>`
- `numeric_constant<T, v>{} * numeric_constant<T, 0>{}` collapses to `null_constant<T>`

Going beyond

- `numeric_constant` can have a `value_category`: `finite`, `infinite`, `nan`, `integer` ...
- We can rewrite all arithmetic rules to optimize during the compilation process: doable in C++23, but easier with reflection and `meta_info` in C++26

Conclusion

- We can have a nice unified interface corresponding to Butcher's Tableau: $a_{ij}, b_j^n, c_i, \beta_j^n$
- Coefficients are easy to specify
- Yet, the formulas can be optimized so that special numeric values do not cause overhead
- Multidimensional access through `std::mdspan` can then be generated for the method's coefficients

Outlooks

Toward a computer algebra system for C++

By combining last year strategies for symbolic computing and ode solvers so that we can have a nice syntax:

```
solve[{gpu}](  
    derivative(y, t) = a * H0 * sqrt(  
        Omega_r0 * pow(a, -4)  
        + Omega_m0 * pow(a, -3)  
        + Omega_k0 * pow(a, -2)  
        + Omega_lambda0  
    ),  
    my_runge_kutta_solver  
)
```

⇒ Goal for next year!

Science outlooks

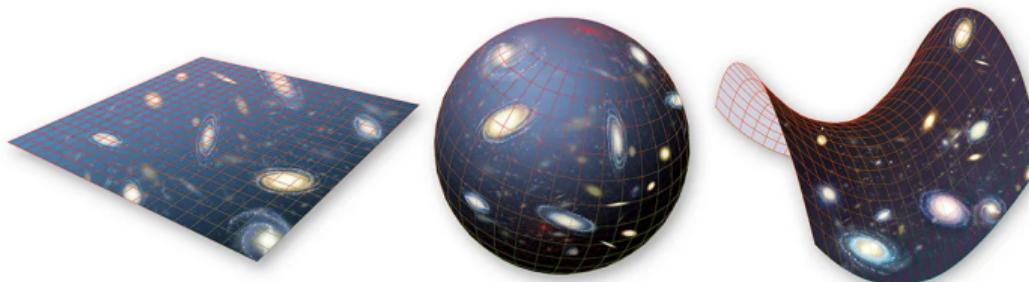
Basic yet interesting cosmological test

Have the same interface to integrate:

- space-time geometry (FLRW equations)
- direct N-body dynamics

for example to check:

- what happens to a N-body system with a global constant curvature?



Conclusion

1 Introduction

2 Firsts steps

3 Context

4 Theoretical foundations

5 Outline of an implementation

6 Conclusion

Summary

Most important lesson in terms of software architecture

- The best software abstractions are derived from well-posed mathematical abstractions
- Conversely, if your problem is not well abstracted it is because solid mathematical foundations are missing

Ordinary Differential Equation solvers

- Good excercise to implement your own: it is not that difficult
- ODE methods have been well abstracted in mathematics: Runge-Kutta (RK), Linear Multistep Methods (LMM), General Linear Methods (GLM)
- Runge-Kutta methods can be represented as a Butcher Tableau
- General Linear Methods matrices A, B, U, V can abstract most common methods

Implementation outline

- Rely on coefficient multiarrays
- Intuitive syntax through expression templates
- Hyjacking arithmetic to remove operations will null coefficients
- Generate integration steps from coefficients

Outlooks

- Continue implementation and combine it with symbolic computing methods
- Interesting scientific use case even with simple integrators

Thank you for your attention

Any question?