

Exploring Physics with C++

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EXPLORING PHYSICS WITH C++

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Preface

Motivacija

- Iako ima knjiga koje koriste C++ kao programski jezik za prezentaciju tehnika numerical computinga, taj C++ je zastarjelog (C-like) stila i ne koristi ni blizu sve mogućnosti modernog C++a
- Što se tiče korištenja softvera za istraživanje fizike, postoji prilično opsežna literatura u kojoj se koriste Matlab i Mathematica, u zadnjih par godina ima i sve više knjiga koje koriste Python u takvu svrhu, ali nema baš takve knjige za C++

Osobno

- Tema me fascinira 30 godina, otkad sam prvi put u ruke uzeo Numerical Recipes in C
- A fascinira me i fizika ❤
- I izvrsna je prilika za re-learning, i fizike i ažuriranje znanja C++a

Osnovni cilj je istražiti različite fizikalne pojave, zakonitosti i generalno različite situacije, koristeći C++ za provođenje numeričkih proračuna

Te uz to opisati i relevantnu fiziku i osnovne tehnike numerical computinga koje će se koristiti

Nekakav početni okvir za raspored po količini sadržaja bi bio: 30% fizike, 40% numerical computing, 30% konkretni C++ kôd

Pregled poglavlja

1. Prva tri – osnovni objekti, algoritmi i vizualizacija
2. Osnovna mehanika – 4, 5, 6, i 7
3. Gravity – 8 i 9
4. Inertial, non-inertial frames and coordinate transformations – 10, 11 i 12
5. Rigid body – 13 i 14
6. Special relativity – 15 i 16
7. Electromagnetism – 17, 18, 19
8. Curves and surfaces – 20
9. General relativity - 21

Acknowledgments

Mater i čaća

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Hopefully, this part will be much, much expanded in the final version

Zahvale contributorima

1. Essential mathematical objects

Where we start from the beginning.

PRELIMINARIES

In this chapter we handle the essentials.

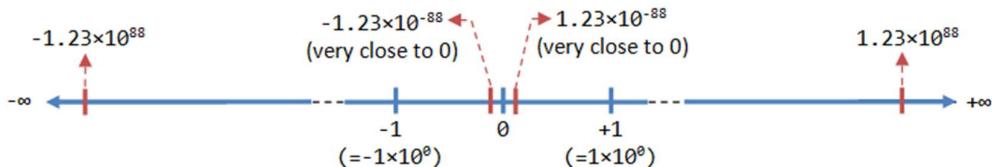
Doing numerics on computer – basics, challenges, pitfalls and traps

Representing numbers

Integers are represented precisely, but hell awaits anyone who steps out of the range of values.

Precision of real representation - about IEEE754, mantissa, exponents, and all that

TODO – nice picture of graphical representation

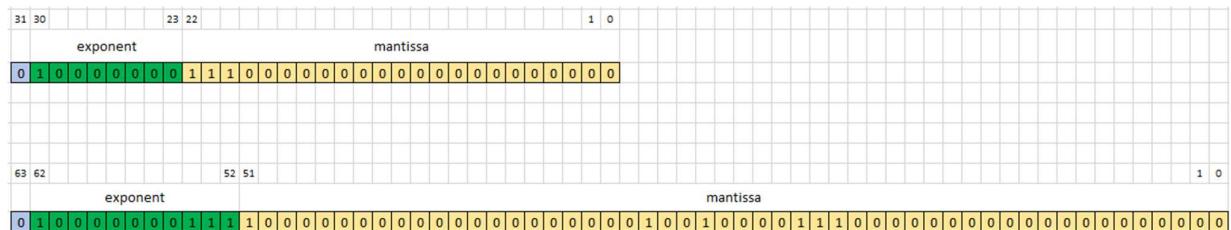
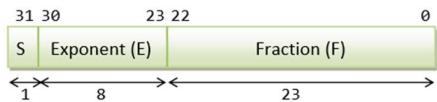


float, double, long double types in standard

representation of special values, in a table like this:

	S	E	F	Value
float	any	1-254	any	$(-1)^S \times 2^{E-127} \times 1.F$
	any	0	nonzero	$(-1)^S \times 2^{-126} \times 0.F*$
	0	0	0	+ 0.0
	1	0	0	- 0.0
	0	255	0	+ ∞
	1	255	0	- ∞
	any	255	nonzero	NaN
double	any	1-2046	any	$(-1)^S \times 2^{E-1023} \times 1.F$
	any	0	nonzero	$(-1)^S \times 2^{-1022} \times 0.F*$
	0	0	0	+ 0.0
	1	0	0	- 0.0
	0	2047	0	+ ∞
	1	2047	0	- ∞
	any	2047	nonzero	NaN

*unnormalized values



Representing PI

Epsilon for float, double, long double (check on different systems – Win, Mac, Linux)

Compare real representation with resolution needed for measuring lengths of different scale in Solar System.

Measure everything in units of A.U. (astronomical units), where 1.0 = 150 million kilometers or 1.0 = 1.5e11 meters.

For example, Earth radius of 6.400 km in this units is equal to 4.27e-5, or 0.0000427 A.U.!

If we want to simulate something that on Earth is on the scale of 1 meter, well, $1\text{ m} = 6,67e-12$, or, to give a visual representation $0.0000000000667\text{ A.U.}$

For this kind of simulation, float is obviously out of the question, but even if we use double precision, we get a resolution of approximately 1 cm

Let's say we want to calculate motion of thrown ball on Pluto, but with a twist, we want to include ALL gravitational influences in Solar system!

Distance Sun – Pluto is 5.9 billion kilometers, or 5.9e12 meters

Using scale where Pluto's center is exactly at 1.00000000, and taking into account Plut's radius of 1188 km, position of point on Pluto's surface (exactly opposite to Sun) is given by 1.000000000201355.

Distance of 1 meter on Pluto's surface is in this scale equal to 1,6949152e-16, which means that even double precision is completely inadequate for modeling this distance.

`__float128`, existing in GCC and as Quad type in Intel C++ Compiler.

Roundoff errors

Happens because of inexact representation of real numbers.

Couple of examples of roundoff errors

Special emphasis on subtraction of similar numbers

TODO – something like this!

Suppose we wish to evaluate the function

$$f(x) = \frac{1 - \cos(x)}{\sin(x)}, \quad (2.7)$$

for small values of x . If we multiply the denominator and numerator with $1 + \cos(x)$ we obtain the equivalent expression

$$f(x) = \frac{\sin(x)}{1 + \cos(x)}. \quad (2.8)$$

If we now choose $x = 0.007$ (in radians) our choice of precision results in

$$\sin(0.007) \approx 0.69999 \times 10^{-2},$$

and

$$\cos(0.007) \approx 0.99998.$$

The first expression for $f(x)$ results in

$$f(x) = \frac{1 - 0.99998}{0.69999 \times 10^{-2}} = \frac{0.2 \times 10^{-4}}{0.69999 \times 10^{-2}} = 0.28572 \times 10^{-2}, \quad (2.9)$$

while the second expression results in

$$f(x) = \frac{0.69999 \times 10^{-2}}{1 + 0.99998} = \frac{0.69999 \times 10^{-2}}{1.99998} = 0.35000 \times 10^{-2}, \quad (2.10)$$

which is also the exact result. In the first expression, due to our choice of precision, we have only one relevant digit in the numerator, after the subtraction. This leads to a loss of precision and a wrong result due to a cancellation of two nearly equal numbers. If we had chosen a precision of six leading digits, both expressions yield the same answer. If we were to evaluate $x \sim \pi$, then the second expression for $f(x)$ can lead to potential losses of precision due to cancellations of nearly equal numbers.

This simple example demonstrates the loss of numerical precision due to roundoff errors, where the number of leading digits is lost in a subtraction of two near equal numbers. The lesson

Calculating roots of quadratic equations!

Usual way of solving:

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$x = \frac{2c}{-b \pm \sqrt{b^2 - 4ac}}$$

Potentially problematic if a or c (or both) are small leading to discriminant that is very close to the value of ' b' !

Correct way:

$$q \equiv -\frac{1}{2} \left[b + \text{sgn}(b) \sqrt{b^2 - 4ac} \right]$$

With roots calculated as:

$$x_1 = \frac{q}{a} \quad \text{and} \quad x_2 = \frac{c}{q}$$

Truncation errors

Round-off error is result of finite number of digits in our real representation and is characteristic of computer hardware.

Truncation error is a characteristic of practical implementation of (numerical) algorithm and it typically occurs as a consequence of applied “discretization” to otherwise continuous quantities, or when we limit infinite series to a finite number of terms.

TODO!

Numerical computing in modern C++

Has a long history, even though it only recently got value of PI properly in the C++ standard

Savior in 90ties as a successor to Fortan

Today it is somewhat “hidden behind the scene”, in low level libraries used by fabulous Python tools

But when the going gets tough ... it is still the best (and almost the only one) choice.

Many plans for C++ 26 standard

But, special functions have been part of the standard since C++17, and still Clang on MacOS doesn't have them.

Essential math headers

Cmath

Complex

Numbers

limits

numerical_limits<> class, and what it gives

But, C++ in its current standard gives only the basics.

Fortunately, there are great numerical libraries, for almost any domain or purpose, and two stand out in their generality and applicability.

GSL – GNU Scientific Library

Link - <https://www.gnu.org/software/gsl/>

Quoting:

The GNU Scientific Library (GSL) is a numerical library for C and C++ programmers. It is free software under the GNU General Public License.

The library provides a wide range of mathematical routines such as random number generators, special functions and least-squares fitting. There are over 1000 functions in total with an extensive test suite.

Unlike the licenses of proprietary numerical libraries, the license of GSL does not restrict scientific cooperation. It allows you to share your programs freely with others.

Wide range of routines:

Complex Numbers	Quasi-Random Sequences	Discrete Hankel Transforms
Roots of Polynomials	Random Distributions	Root-Finding
Special Functions	Statistics	Minimization
Vectors and Matrices	Histograms	Least-Squares Fitting
Permutations	N-Tuples	Physical Constants
Sorting	Monte Carlo Integration	IEEE Floating-Point
BLAS Support	Simulated Annealing	Discrete Wavelet Transforms
Linear Algebra	Differential Equations	Basis splines
Eigenvalues	Interpolation	Running Statistics
Fast Fourier Transforms	Numerical Differentiation	Sparse Matrices and Linear
Quadrature	Chebyshev Approximation	Algebra
Random Numbers	Series Acceleration	

C oriented!

Mostly you are working with pointers to C structs, allocated (mostly) on the heap.

Rich set of C-like manipulation routines for vectors, matrices, permutations, that usually look like this:

```
gsl_vector *gsl_vector_alloc(size_t n)
```

```
double gsl_vector_get(const gsl_vector *v, const size_t i)
```

```
int gsl_vector_add(gsl_vector *a, const gsl_vector *b)
```

```
gsl_matrix *gsl_matrix_alloc(size_t n1, size_t n2)
```

```
int gsl_matrix_transpose_memcpy(gsl_matrix *dest, const gsl_matrix *src)
```

Simple example of adaptive integration of following function, which has an algebraic-logarithmic singularity at the origin:

$$\int_0^1 x^{-1/2} \log(x) dx = -4$$

Looks like this:

```

#include <stdio.h>
#include <math.h>
#include <gsl/gsl_integration.h>

double f (double x, void * params) {
    double alpha = *(double *) params;
    double f = log(alpha*x) / sqrt(x);
    return f;
}

int
main (void)
{
    gsl_integration_workspace * w
        = gsl_integration_workspace_alloc (1000);

    double result, error;
    double expected = -4.0;
    double alpha = 1.0;

    gsl_function F;
    F.function = &f;
    F.params = &alpha;

    gsl_integration_qags (&F, 0, 1, 0, 1e-7, 1000,
                         w, &result, &error);

    printf ("result      = % .18f\n", result);
    printf ("exact result = % .18f\n", expected);
    printf ("estimated error = % .18f\n", error);
    printf ("actual error   = % .18f\n", result - expected);
    printf ("intervals     = %zu\n", w->size);

    gsl_integration_workspace_free (w);

    return 0;
}

```

And example of solving Van der Pol differential equation

$$u''(t) + \mu u'(t)(u(t)^2 - 1) + u(t) = 0$$

When it is decoupled to two first order equations

$$\begin{aligned} u' &= v \\ v' &= -u + \mu v(1 - u^2) \end{aligned}$$

Looks like this, where we define also Jacobian for this system.

```

int func (double t, const double y[], double f[], void *params)
{
    /*(void)(t); /* avoid unused parameter warning */
    double mu = *(double *)params;

    f[0] = y[1];
    f[1] = -y[0] - mu*y[1]*(y[0]*y[0] - 1);

    return GSL_SUCCESS;
}

```

Jacobian

```

int jac (double t, const double y[], double *dfdy, double dfdt[], void *params)
{
    /*(void)(t); /* avoid unused parameter warning */
    double mu = *(double *)params;

    gsl_matrix_view dfdy_mat = gsl_matrix_view_array (dfdy, 2, 2);
    gsl_matrix *m = &dfdy_mat.matrix;

    gsl_matrix_set (m, 0, 0, 0.0);
    gsl_matrix_set (m, 0, 1, 1.0);
    gsl_matrix_set (m, 1, 0, -2.0*mu*y[0]*y[1] - 1.0);
    gsl_matrix_set (m, 1, 1, -mu*(y[0]*y[0] - 1.0));

    dfdt[0] = 0.0;
    dfdt[1] = 0.0;

    return GSL_SUCCESS;
}

```

Solving it with driver program, where we are using Prince-Dormand 8th order method to obtain solution (parameter ‘gsl_odeiv2_step_rk8pd’):

```

void gsl_van_der_pol (void)
{
    double mu = 10;
    gsl_odeiv2_system sys = {func, jac, 2, &mu};

    gsl_odeiv2_driver * driver =
        gsl_odeiv2_driver_alloc_y_new (&sys, gsl_odeiv2_step_rk8pd, 1e-6, 1e-6, 0.0);

    int i;
    double t = 0.0, t1 = 100.0;
    double y[2] = { 1.0, 0.0 };

    for (i = 1; i <= 100; i++)
    {
        double ti = i * t1 / 100.0;
        int status = gsl_odeiv2_driver_apply (driver, &t, ti, y);

        if (status != GSL_SUCCESS)
        {
            printf ("error, return value=%d\n", status);
            break;
        }

        printf ("% .5e % .5e % .5e\n", t, y[0], y[1]);
    }

    gsl_odeiv2_driver_free (driver);
}

```

Boost

Link - <https://www.boost.org/>

Premiere C++ library, if somewhat over-bloated (700+ Mb when extracted on hard disk).

Still, math functionality is mostly in standard Boost style, implemented solely in easily included headers ... and there is much to include.

- Math library – special functions, polynomials, rational functions, root finding and function minimization, interpolation and numerical differentiation and integration
- Geometry – various geometry algorithms
- Multiprecision – support for `__float128` type
- Odeint – solving differential equations
- QVM – quaternions, vectors, matrices
- uBLAS – linear algebra routines

Example of defining stiff Van der Pol system:

```
const double mu = 1000.0;

typedef boost::numeric::ublas::vector< double > vector_type;
typedef boost::numeric::ublas::matrix< double > matrix_type;

struct vdp_stiff
{
    void operator()(const vector_type& x, vector_type& dxdt, double t)
    {
        dxdt[0] = x[1];
        dxdt[1] = -x[0] - mu * x[1] * (x[0] * x[0] - 1.0);
    }
};

struct vdp_stiff_jacobi
{
    void operator()(const vector_type& x, matrix_type& J, const double& t, vector_type& dfdt)
    {
        J(0, 0) = 0.0;
        J(0, 1) = 1.0;
        J(1, 0) = -1.0 - 2.0 * mu * x[0] * x[1];
        J(1, 1) = -mu * (x[0] * x[0] - 1.0);

        dfdt[0] = 0.0;
        dfdt[1] = 0.0;
    }
};
```

And solving it using Rosenbrock method:

```
void boost_van_der_pol_stiff()
{
    vector_type x(2);
    srand(time(NULL));

    // initial conditions - set to random
    for (int i = 0; i < 2; i++)
        x[i] = (1.0 * rand()) / RAND_MAX;

    size_t num_of_steps = integrate_const(make_dense_output< rosenbrock4< double >> (1.0e-6, 1.0e-6),
                                           make_pair(vdp_stiff(), vdp_stiff_jacobi()),
                                           x, 0.0, 1000.0, 1.0,
                                           cout << phoenix::arg_names::arg2 << " "
                                               << phoenix::arg_names::arg1[0] << " "
                                               << phoenix::arg_names::arg1[1] << "\n"
                                           );
    clog << num_of_steps << endl;
}
```

Overview of other C++ numerical libraries of note

There are many, many, many

Wikipedia page gives good overview - [LINK](#)

Some of those of a more “general” orientation and applicability are:

Eigen - <https://eigen.tuxfamily.org/>

Armadillo - <https://arma.sourceforge.net/>

ALGLIB - <https://www.alglib.net/>

Blaze - <https://bitbucket.org/blaze-lib>

Trilinos - <https://trilinos.github.io/>

Starting our own Minimal Math Library

Why not just use Boost or GSL?

- We will be using them ... in certain situations
- Learning by implementing
- Creating general math library that is versatile and easily usable for physical simulations

And that also has basic mathematical objects directly modelled (in today's parlance, you could say it is "opinionated")

C++20 is our starting point, but it should be quite easy customizing everything for C++14 and C++17.

MMLBase.h

This will be the base header for our library.

Starting with necessary headers we need to include

```
#include <stdexcept>
#include <initializer_list>
#include <algorithm>
#include <memory>
#include <functional>

#include <string>
#include <vector>
#include <fstream>
#include <iostream>
#include <iomanip>

#include <cmath>
#include <limits>
#include <complex>
#include <numbers>
```

Following good programming practice, all our code will be within namespace MML, and we start with some global paths for our visualizers.

```
namespace MML
{
    // Global paths for Visualizers
    static const std::string MML_GLOBAL_PATH = "E:/Projects/MinimalMathLibrary";
    //static const std::string MML_GLOBAL_PATH = "/usr/zvanjak/projects/MinimalMathLibrary";

    static const std::string MML_PATH_ResultFiles = MML_GLOBAL_PATH +
        "/results/";

    static const std::string MML_PATH_RealFuncViz = MML_GLOBAL_PATH +
        "/tools/visualizers/real_function_visualizer/MML_RealFunctionVisualizer.exe";
    static const std::string MML_PATH_SurfaceViz = MML_GLOBAL_PATH +
        "/tools/visualizers/scalar_function_2d_visualizer/MML_ScalarFunction2Visualizer.exe";
    static const std::string MML_PATH_ParametricCurveViz = MML_GLOBAL_PATH +
        "/tools/visualizers/parametric_curve_visualizer/MML_ParametricCurveVisualizer.exe";
    static const std::string MML_PATH_VectorFieldViz = MML_GLOBAL_PATH +
        "/tools/visualizers/vector_field_visualizer/MML_VectorFieldVisualizer.exe";
}
```

Continuing with some basics

```
template<class Type>
static Real Abs(const Type& a)
{
    return std::abs(a);
}

template<class Type>
static Real Abs(const std::complex<Type>& a)
{
    return hypot(a.real(), a.imag());
}

inline bool isWithinAbsPrec(Real a, Real b, Real eps)
{
    return std::abs(a - b) < eps;
}

inline bool isWithinRelPrec(Real a, Real b, Real eps)
{
    return std::abs(a - b) < eps * std::max(Abs(a), Abs(b));
}
```

Solving “inconvenience” that is a missing power operator in C++.

```
template<class T> inline T POW2(const T a) { const T t = a; return t * t; }
template<class T> inline T POW3(const T a) { const T t = a; return t * t * t; }
template<class T> inline T POW4(const T a) { const T t = a; return t * t * t * t; }
```

Solvers for quadratic, cubic and quartic equations.

```
// a * x^2 + b * x + c = 0
static int SolveQuadratic(Real a, Real b, Real c,
    Complex& x1, Complex& x2) { ... }

static void SolveQuadratic(const Complex& a, const Complex& b, const Complex& c,
    Complex& x1, Complex& x2) { ... }

// Solving cubic equation a * x^3 + b * x^2 + c * x + d = 0
static int SolveCubic(Real a, Real b, Real c, Real d,
    Complex& x1, Complex& x2, Complex& x3) { ... }

// FIX - Solving quartic equation a * x^4 + b * x^3 + c * x^2 + d * x + e = 0
static void SolveQuartic(Real a, Real b, Real c, Real d, Real e,
    Complex& x1, Complex& x2, Complex& x3, Complex& x4) { ... }
```

Constants

```
namespace Constants
{
    static inline const Real PI = std::numbers::pi;
    static inline const Real INV_PI = std::numbers::inv_pi;
    static inline const Real INV_SQRTPI = std::numbers::inv_sqrt(pi);

    static inline const Real E = std::numbers::e;
    static inline const Real LN2 = std::numbers::ln2;
    static inline const Real LN10 = std::numbers::ln10;

    static inline const Real SQRT2 = std::numbers::sqrt2;
    static inline const Real SQRT3 = std::numbers::sqrt3;

    static inline const Real Epsilon = std::numeric_limits<Real>::epsilon();
    static inline const Real PositiveInf = std::numeric_limits<Real>::max();
    static inline const Real NegativeInf = -std::numeric_limits<Real>::max();
}
```

In Defaults namespace we first define some default values for objects output

TODO – expand and improve

```
namespace Defaults
{
    // Output defaults
    static int VectorPrintWidth = 15;
    static int VectorPrintPrecision = 10;
    static int VectorNPrintWidth = 15;
    static int VectorNPrintPrecision = 10;
```

Then we define some defaults for precision of numerical operations.

```
////////// Default precisions //////////
// Use the precision values based on the Real type
static inline const Real ComplexAreEqualTolerance = PrecisionValues<Real>::ComplexAreEqualTolerance;
static inline const Real ComplexAreEqualAbsTolerance = PrecisionValues<Real>::ComplexAreEqualAbsTolerance;
static inline const Real VectorIsEqualTolerance = PrecisionValues<Real>::VectorIsEqualTolerance;
static inline const Real MatrixIsEqualTolerance = PrecisionValues<Real>::MatrixIsEqualTolerance;

static inline const Real Pnt2CartIsEqualTolerance = PrecisionValues<Real>::Pnt2CartIsEqualTolerance;
static inline const Real Pnt2PolarIsEqualTolerance = PrecisionValues<Real>::Pnt2PolarIsEqualTolerance;
static inline const Real Pnt3CartIsEqualTolerance = PrecisionValues<Real>::Pnt3CartIsEqualTolerance;
static inline const Real Pnt3SphIsEqualTolerance = PrecisionValues<Real>::Pnt3SphIsEqualTolerance;
static inline const Real Pnt3CylIsEqualTolerance = PrecisionValues<Real>::Pnt3CylIsEqualTolerance;

static inline const Real Vec2CartIsEqualTolerance = PrecisionValues<Real>::Vec2CartIsEqualTolerance;
static inline const Real Vec3CartIsEqualTolerance = PrecisionValues<Real>::Vec3CartIsEqualTolerance;
static inline const Real Vec3CartIsParallelTolerance = PrecisionValues<Real>::Vec3CartIsParallelTolerance;

static inline const Real Line3DIsPerpendicularTolerance = PrecisionValues<Real>::Line3DIsPerpendicularTolerance;
static inline const Real Line3DIsParallelTolerance = PrecisionValues<Real>::Line3DIsParallelTolerance;
static inline const Real Plane3DIsPointOnPlaneTolerance = PrecisionValues<Real>::Plane3DIsPointOnPlaneTolerance;

static inline const Real IsMatrixSymmetricTolerance = PrecisionValues<Real>::IsMatrixSymmetricTolerance;
static inline const Real IsMatrixDiagonalTolerance = PrecisionValues<Real>::IsMatrixDiagonalTolerance;
static inline const Real IsMatrixUnitTolerance = PrecisionValues<Real>::IsMatrixUnitTolerance;
static inline const Real IsMatrixOrthogonalTolerance = PrecisionValues<Real>::IsMatrixOrthogonalTolerance;
```

Customized for different ‘Real’ types with the use of template specialization.

General template.

```
// Template struct for precision values
template<typename T>
struct PrecisionValues;
```

Specialization for float type:

```
template<>
struct PrecisionValues<float>
{
    static constexpr float ComplexAreEqualTolerance = 1e-6f;
    static constexpr float ComplexAreEqualAbsTolerance = 1e-6f;

    static constexpr float MatrixIsEqualTolerance = 1e-6f;
    static constexpr float VectorIsEqualTolerance = 1e-6f;
```

And likewise (with different values) for double and long double types.

We will also specify a list of all standard math functions, available in almost every C++ compiler today

```
static inline Real Sin(Real x) { return sin(x); }
static inline Real Cos(Real x) { return cos(x); }
static inline Real Sec(Real x) { return 1.0 / cos(x); }
static inline Real Csc(Real x) { return 1.0 / sin(x); }
static inline Real Tan(Real x) { return tan(x); }
static inline Real Ctg(Real x) { return 1.0 / tan(x); }

static inline Real Exp(Real x) { return exp(x); }
static inline Real Log(Real x) { return log(x); }
static inline Real Log10(Real x){ return log10(x); }
static inline Real Sqrt(Real x) { return sqrt(x); }
static inline Real Pow(Real x, Real y) { return pow(x, y); }

static inline Real Sinh(Real x) { return sinh(x); }
static inline Real Cosh(Real x) { return cosh(x); }
static inline Real Sech(Real x) { return 1.0 / cosh(x); }
static inline Real CsCh(Real x) { return 1.0 / sinh(x); }
static inline Real Tanh(Real x) { return tanh(x); }
static inline Real Ctgh(Real x) { return 1.0 / tanh(x); }

static inline Real Asin(Real x) { return asin(x); }
static inline Real Acos(Real x) { return acos(x); }
static inline Real Atan(Real x) { return atan(x); }

static inline Real Asinh(Real x) { return asinh(x); }
static inline Real Acosh(Real x) { return acosh(x); }
static inline Real Atanh(Real x) { return atanh(x); }
```

And a list of special functions, available from in C++17 standard (but still lacking in some compilers).

MSVC & gcc handle these correctly, but Clang is lacking, or to be more precise, Clang on MacOS (TODO – investigate properly)

```
static inline Real Erf(Real x) { return std::erf(x); }
static inline Real Erfc(Real x) { return std::erfc(x); }

static inline Real TGamma(Real x) { return std::tgamma(x); }
static inline Real LGamma(Real x) { return std::lgamma(x); }
static inline Real RiemannZeta(Real x) { return std::riemann_zeta(x); }
static inline Real Comp_ellint_1(Real x) { return std::comp_ellint_1(x); }
static inline Real Comp_ellint_2(Real x) { return std::comp_ellint_2(x); }

static inline Real Hermite(unsigned int n, Real x) { return std::hermite(n, x); }
static inline Real Legendre(unsigned int n, Real x) { return std::legendre(n, x); }
static inline Real Laguerre(unsigned int n, Real x) { return std::laguerre(n, x); }
static inline Real SphBessel(unsigned int n, Real x) { return std::sph_bessel(n, x); }
static inline Real SphLegendre(int n1, int n2, Real x) { return std::sph_legendre(n1, n2, x); }
```

MMLExceptions.h

Even though having exceptions in our code exacts (quite) a small runtime penalty, it is a small price for having dependable way of handling exceptional situations.

No deep inheritance hierarchies.

Each exception is inherited from C++ standard exception that mostly resembles the problem and tries to report as much information as possible about possible causes.

Set of classes defined in MMLErrors.h

```
namespace MML
{
    ////////////// Vector error exceptions /////////////
    class VectorInitializationError { ... };
    class VectorDimensionError { ... };
    class VectorAccessBoundsError { ... };

    ////////////// Matrix error exceptions /////////////
    class MatrixAllocationError { ... };
    class MatrixAccessBoundsError { ... };
    class MatrixDimensionError { ... };
    class SingularMatrixError { ... };

    ////////////// Integration exceptions /////////////
    class IntegrationTooManySteps { ... };

    ////////////// Interpolation exceptions /////////////
    class RealFuncInterpInitError { ... };

    ////////////// Tensor exceptions /////////////
    class TensorCovarContravarNumError { ... };
    class TensorCovarContravarArithmeticError { ... };
    class TensorIndexError { ... };

    ////////////// Root finding exceptions /////////////
    class RootFindingError { ... };

    ////////////// ODE solver exceptions /////////////
    class ODESolverError { ... };
}
```

Running code and examples

All code presented in this book is available on Github (<https://github.com/zvanjak/ExploringPhysicsWithCpp>)

Using Visual studio code with standard extensions for C++ development

Working with different compilers – tested on MSVC, Clang, gcc

Tested on different platforms – Windows, Ubuntu, Mac.

VECTOR – “THE WORKHORSE”

What is a vector?

Can represent almost anything, and in our physics investigations we'll use it to represent Cartesian and spherical vectors, momentum and angular momentum, ...

but in essence, it is an array of numbers, real or complex, of some determined size and it is present in almost all numerical calculations.

Templated – so it can contain any kind of type

Two types.

- Runtime size
- Compile time size

Vector<Type> - runtime size

Represents (mathematical!) vector of dynamically defined size, and it is basically a wrapper around std::vector<>.

Delegation, not inheritance!

As we will be at the same time restricting set of operations available from std::vector<> and extending that set with some mathematical operations, not present in std::vector<>.

<https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/mml/base/Vector.h>

```
template<class Type>
class Vector
{
private:
    std::vector<Type> _elems;

public:
    typedef Type value_type;      // make T available externally
    ////////////////////////////// Constructors //////////////////////////////
    Vector() {}
    explicit Vector(int n) { ... }
    explicit Vector(int n, const Type &val) { ... }
    explicit Vector(int n, Type* vals) { ... }
    explicit Vector(std::vector<Type> values) : _elems(values) {}
    explicit Vector(std::initializer_list<Type> list) : _elems(list) {}
```

Basic set of standard constructors.

For accessing element, we implement two approaches – with and without bounds checking.

```

/////////// Accessing elements //////////
inline Type& operator[](int n) { return _elems[n]; }
inline const Type& operator[](int n) const { return _elems[n]; }

// checked access
Type& at(int n) {
    if(n < 0 || n >= size())
        throw VectorDimensionError("Vector::at - index out of bounds", size(), n);
    else
        return _elems[n];
}
Type at(int n) const {
    if(n < 0 || n >= size())
        throw VectorDimensionError("Vector::at - index out of bounds", size(), n);
    else
        return _elems[n];
}

```

Set of implemented arithmetic operators.

```

/////////// Arithmetic operators //////////
Vector operator-() const { ... }

Vector operator+(const Vector& b) const { ... }
Vector& operator+=(const Vector& b) { ... }
Vector operator-(const Vector& b) const { ... }
Vector& operator-=(const Vector& b) { ... }

Vector operator*(Type b) { ... }
Vector& operator*=(Type b) { ... }
Vector operator/(Type b) { ... }
Vector& operator/=(Type b) { ... }

friend Vector operator*(Type a, const Vector& b) { ... }

```

Operations for testing equality

```

/////////// Testing equality //////////
bool operator==(const Vector& b) const { ... }
bool operator!=(const Vector& b) const { ... }
bool IsEqualTo(const Vector& b, Real eps = Defaults::VectorEqualityPrecision) const { ... }
bool IsNullVec() const { ... }

```

Calculating vector norm

```

/////////// Operations //////////
Real NormL1() const { ... }
Real NormL2() const { ... }
Real NormLInf() const { ... }

```

I/O for vectors

```

/////////// I/O //////////
std::ostream& Print(std::ostream& stream, int width, int precision) const { ... }
std::ostream& Print(std::ostream& stream, int width, int precision, Real zeroThreshold) const { ... }
std::ostream& PrintLine(std::ostream& stream, const std::string &msg, int width, int precision) const { ... }

std::string to_string(int width, int precision) const { ... }
friend std::ostream& operator<<(std::ostream &stream, const Vector &a) { ... }

```

VectorN<Type, N> - compile-time size

Vector with statically defined size.

Needed mostly in its 2D, 3D or 4D incarnations, where it will be used as base class for some specific implementations.

Has mostly the same functionality as Vector, with obvious difference in data declaration and minor differences in constructors.

<https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/mml/base/VectorN.h>

```
template<class Type, int N> <T> Provide sample template arguments for IntelliSense ✓
class VectorN
{
protected:
    Type _val[N] = { 0 };

public:
    typedef Type value_type;      // make T available externally

    //////////////////// Constructors and destructor ///////////////////
    VectorN() {}
    explicit VectorN(const Type& init_val) { ... }
    explicit VectorN(std::initializer_list<Type> list) { ... }
    explicit VectorN(std::vector<Type> list) { ... }
    explicit VectorN(Type* vals) { ... }
```

Starting our Utils namespace

Utility namespace with static helpers of various kinds and stuff that even though it is closely associated with Vector class, doesn't merit inclusion as a pure member.

In some cases, it is actually impossible to preserve semantics, as in the case of ScalarProduct() helper function where implementation for Real and Complex types is different.

```
////////////////// Vector helpers //////////////////
static bool AreEqual(const Vector<Real> &a, const Vector<Real> &b,
                     Real eps = Defaults::VectorIsEqualTolerance) { ... }
static bool AreEqual(const Vector<Complex>& a, const Vector<Complex>& b,
                     Real eps = Defaults::ComplexAreEqualTolerance) { ... }
static bool AreEqualAbs(const Vector<Complex>& a, const Vector<Complex>& b,
                       Real eps = Defaults::ComplexAreEqualAbsTolerance) { ... }

static Real ScalarProduct(const Vector<Real>& a, const Vector<Real>& b) { ... }
static Complex ScalarProduct(const Vector<Complex>& a, const Vector<Complex>& b) { ... }
static Real VectorsAngle(const Vector<Real>& a, const Vector<Real>& b) { ... }

static Vector<Real> VectorProjectionParallelTo(const Vector<Real>& orig, const Vector<Real>& b) { ... }
static Vector<Real> VectorProjectionPerpendicularTo(const Vector<Real>& orig, const Vector<Real>& b) { ... }

template<int N>
static Real ScalarProduct(const VectorN<Real, N> &a, const VectorN<Real, N> &b) { ... }
template<int N>
static Complex ScalarProduct(const VectorN<Complex, N>& a, const VectorN<Complex, N>& b) { ... }

template<int N>
static Real VectorsAngle(const VectorN<Real, N> &a, const VectorN<Real, N> &b) { ... }
```

Unfortunately, mixing operations between different Vector types requires special functions.

```
////////////////// Vector<Complex> - Vector<Real> operations //////////////////
static Vector<Complex> AddVec(const Vector<Complex>& a, const Vector<Real>& b){{ ... }};
static Vector<Complex> AddVec(const Vector<Real>& a, const Vector<Complex>& b){{ ... }};

static Vector<Complex> SubVec(const Vector<Complex>& a, const Vector<Real>& b){{ ... }};
static Vector<Complex> SubVec(const Vector<Real>& a, const Vector<Complex>& b){{ ... }};
```

Example usage

Example with vectors and its operations.

https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/Chapter_01_basic_objects/demo_vector.cpp

```
// REAL vectors
Vector<Real>    vec1(5);           // init vector with 5 elements
Vector<Real>    vec2(3, 3.14159);   // init with constant value
Vector<Real>    vec3({ 1.5, -2.1, 0.48 }); // init with list of values

// using defined aliases (typedefs)
VectorDbl    vec4(vec3);          // init with copy ctor
VecD        vec5 = vec2;          // init with assignment

// initializing from std::vector and C/C++ array
std::vector<Real> std_vec{ -1.0, 5.0, -2.0 };
float    arr[5] = { -1.0, 5.0, -2.0, 10.0, 4.0 };

Vector<Real>    vec6(std_vec);    // init with std::vector<>
VectorFlt     vec7(5, arr);       // init with C/C++ array

// COMPLEX vectors
Vector<Complex> vec_c1({ 1.0, 2.0, 3.0 }); // init with list of real values
VecC        vec_c2({ Complex(1,1),
                    Complex(-1,2),
                    Complex(2, -0.5) }); // init with list of complex values

// vector operations
Vector<Real> v1 = vec2 / 2.0 - 1.5 * vec6;
v1 /= vec4.NormL2();

Vector<Complex> v2 = vec_c1 + vec_c2 * Complex(0.5, -1.5);

Real    scalar_prod = Utils::ScalarProduct(vec2, vec3);
Complex scalar_prod_cmplx = Utils::ScalarProduct(vec_c1, vec_c2);
```

MATRIX – “THE OMNIPRESENT”

Used everywhere ...

Matrix<Type> - runtime size

Standard Matrix object with size defined at runtime, ie. at construction time.

Space for storing elements is allocated as contiguous block (not on a per row basis).

<https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/mml/base/Matrix.h>

Data and private parts.

```
template<class Type>
class Matrix
{
private:
    int _rows;
    int _cols;
    Type** _data;

    void Init(int rows, int cols){ ... }
    void ReleaseMemory(){ ... }
```

Set of available constructors.

```
explicit Matrix() : _rows(0), _cols(0), _data{ nullptr } {}
explicit Matrix(int rows, int cols){ ... }
explicit Matrix(int rows, int cols, const Type& val){ ... }
// useful if you have a pointer to continuous 2D array (can be in row-, or column-wise memory layout)
explicit Matrix(int rows, int cols, Type* val, bool isRowWise = true){ ... }
// in strict mode, you must supply ALL necessary values for complete matrix initialization
explicit Matrix(int rows, int cols, std::initializer_list<Type> values, bool strictMode = true){ ... }

Matrix(const Matrix& m){ ... }
// creating submatrix from given matrix 'm'
Matrix(const Matrix& m, int ind_row, int ind_col, int row_num, int col_num){ ... }
Matrix(Matrix&& m){ ... }
~Matrix(){ ... }
```

Some basic operations

```
void Resize(int rows, int cols, bool preserveElements = false){ ... }

Vector<Type> VectorFromRow(int rowInd) const{ ... }
Vector<Type> VectorFromColumn(int colInd) const{ ... }
Vector<Type> VectorFromDiagonal() const{ ... }
```

Some more basics stuff, and some manipulation routines.

```
inline int RowNum() const { return _rows; }
inline int ColNum() const { return _cols; }

static Matrix GetUnitMatrix(int dim) { ... }
void MakeUnitMatrix(void) { ... }

Matrix GetLower(bool includeDiagonal = true) const { ... }
Matrix GetUpper(bool includeDiagonal = true) const { ... }

void InitRowWithVector(int rowInd, const Vector<Type>& vec) { ... }
void InitColWithVector(int colInd, const Vector<Type>& vec) { ... }

void SwapRows(int k, int l) { ... }
void SwapCols(int k, int l) { ... }
```

Functions for calculating various matrix properties.

TODO – separate Norm calculations, and give math definitions

```
////////////////// Matrix properties ///////////////////
bool IsUnit(double eps = Defaults::IsMatrixUnitPrecision) const { ... }
bool IsDiagonal(double eps = Defaults::IsMatrixDiagonalPrecision) const { ... }
bool IsDiagDominant() const { ... }
bool IsSymmetric() const { ... }
bool IsAntiSymmetric() const { ... }

Real NormL1() const { ... }
Real NormL2() const { ... }
Real NormLInf() const { ... }
```

Assignment and access operators.

```
////////////////// Assignment operators ///////////////////
Matrix& operator=(const Matrix& m) { ... }
Matrix& operator=(Matrix&& m) { ... }

////////////////// Access operators ///////////////////
inline Type* operator[](int i) { return _data[i]; }
inline const Type* operator[](const int i) const { return _data[i]; }

inline Type operator()(int i, int j) const { return _data[i][j]; }
inline Type& operator()(int i, int j) { return _data[i][j]; }

// version with checked access
Type at(int i, int j) const { ... }
Type& at(int i, int j) { ... }
```

Two ways to check for equality – exact, implemented with operators == and !=, and the other one where you can specify wanted precision

```
////////////////// Equality operations ///////////////////
bool operator==(const Matrix& b) const { ... }
bool operator!=(const Matrix& b) const { ... }

bool IsEqualTo(const Matrix<Type>& b, Type eps = Defaults::MatrixEqualityPrecision) const { ... }
static bool AreEqual(const Matrix& a, const Matrix& b, Type eps = Defaults::MatrixEqualityPrecision)
```

Standard set of arithmetic operators.

```
/////////////////////////////          Arithmetic operators          ///////////////////
Matrix operator-() const { ... }

Matrix operator+(const Matrix& b) const { ... }
Matrix& operator+=(const Matrix& b) { ... }
Matrix operator-(const Matrix& b) const { ... }
Matrix& operator-=(const Matrix& b) { ... }
Matrix operator*(const Matrix& b) const { ... }

Matrix operator*(const Type &b) const { ... }
Matrix& operator*=(const Type &b) { ... }
Matrix operator/(const Type &b) const { ... }
Matrix& operator/=(const Type &b) { ... }

Vector<Type> operator*(const Vector<Type>& b) const { ... }

friend Matrix operator*(const Type &a, const Matrix<Type>& b) { ... }
friend Vector<Type> operator*(const Vector<Type>& a, const Matrix<Type>& b) { ... }
```

Basic operations, where matrix inversion is performed by using Gauss-Jordan elimination with pivoting.

```
/////////////////////////////          Trace, Inverse & Transpose          ///////////////////
Type Trace() const { ... }

void Invert() { ... }
Matrix GetInverse() const { ... }

void Transpose() { ... }
Matrix GetTranspose() const { ... }
```

Printing to console and working with files

```
/////////////////////////////          I/O          ///////////////////
void Print(std::ostream& stream, int width, int precision) const { ... }
void Print(std::ostream& stream, int width, int precision, Real zeroThreshold) const { ... }

friend std::ostream& operator<<(std::ostream& stream, const Matrix& a) { ... }
std::string to_string(int width, int precision) const { ... }

static bool LoadFromFile(std::string inFile, Matrix& mat) { ... }
static bool SaveToFile(const Matrix& mat, std::string inFile) { ... }
```

MatrixNM<Type, N, M> - compile-time size

Different from Matrix in additional template parameters, and internal structure, but basically the same in functionality.

<https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/mml/base/MatrixNM.h>

```
template <class Type, int N, int M>
class MatrixNM
{
public:
    Type _vals[N][M] = { {0} };

public:
    typedef Type value_type; // make T available externally

    ////////////////////////////// Constructors /////////////////////
    MatrixNM() {}
    MatrixNM(std::initializer_list<Type> values) { ... }
    MatrixNM(const MatrixNM& m) { ... }
    MatrixNM(const Type& m) { ... }
```

Extending Utils namespace with matrix helpers

Similarly to Vector helpers, we add to our BaseUtils.h header various helpers for Matrix classes.

```
////////////////// Creating Matrix from Vector //////////////////
template<class Type> static Matrix<Type> RowMatrixFromVector(const Vector<Type>& b) { ... }
template<class Type> static Matrix<Type> ColumnMatrixFromVector(const Vector<Type>& b) { ... }
template<class Type> static Matrix<Type> DiagonalMatrixFromVector(const Vector<Type>& b) { ... }

template<class Type, int N> MatrixNM<Type, 1, N> RowMatrixFromVector(const VectorN<Type>, N& b) { ... }
template<class Type, int N> MatrixNM<Type, N, 1> ColumnMatrixFromVector(const VectorN<Type>, N& b) { ... }
template<class Type, int N> MatrixNM<Type, N, N> DiagonalMatrixFromVector(const VectorN<Type>, N& b) { ... }

////////////////// Matrix helpers ///////////////////
template<class Type> static Matrix<Type> Commutator(const Matrix<Type>& a, const Matrix<Type>& b) { ... }
template<class Type> static Matrix<Type> AntiCommutator(const Matrix<Type>& a, const Matrix<Type>& b) { ... }

template<class Type>
static void MatrixDecomposeToSymAntisym(const Matrix<Type>& orig,
                                         Matrix<Type>& outSym,
                                         Matrix<Type>& outAntiSym) { ... }

////////////////// Matrix functions ///////////////////
template<class Type> static Matrix<Type> Exp(const Matrix<Type>& a, int n = 10) { ... }
template<class Type> static Matrix<Type> Sin(const Matrix<Type>& a, int n = 10) { ... }
template<class Type> static Matrix<Type> Cos(const Matrix<Type>& a, int n = 10) { ... }
```

Calculating different matrix properties

```
////////// Real matrix helpers //////////
static bool IsOrthogonal(const Matrix<Real>& mat, double eps = Defaults::IsMatrixOrthogonalPrecision)

////////// Complex matrix helpers //////////
static Matrix<Real> GetRealPart(const Matrix<Complex>& a) { ... }
static Matrix<Real> GetImagPart(const Matrix<Complex>& a) { ... }

static Matrix<Complex> GetConjugateTranspose(const Matrix<Complex>& mat) { ... }
static Matrix<Complex> CmplxMatFromRealMat(const Matrix<Real>& mat) { ... }

static bool IsComplexMatReal(const Matrix<Complex>& mat) { ... }
static bool IsHermitian(const Matrix<Complex>& mat) { ... }
static bool IsUnitary(const Matrix<Complex>& mat) { ... }
```

Set of functions for performing arithmetic between Real and Complex matrices

```
////////// Matrix<Complex> - Matrix<Real> operations //////////
static Matrix<Complex> AddMat(const Matrix<Complex>& a, const Matrix<Real>& b) { ... }
static Matrix<Complex> AddMat(const Matrix<Real>& a, const Matrix<Complex>& b) { ... }

static Matrix<Complex> SubMat(const Matrix<Complex>& a, const Matrix<Real>& b) { ... }
static Matrix<Complex> SubMat(const Matrix<Real>& a, const Matrix<Complex>& b) { ... }

static Matrix<Complex> MulMat(const Complex& a, const Matrix<Real>& b) { ... }
static Matrix<Complex> MulMat(const Matrix<Real>& a, const Complex& b) { ... }

static Matrix<Complex> MulMat(const Matrix<Complex>& a, const Matrix<Real>& b) { ... }
static Matrix<Complex> MulMat(const Matrix<Real>& a, const Matrix<Complex>& b) { ... }

static Vector<Complex> MulMatVec(const Matrix<Real>& a, const Vector<Complex>& b) { ... }
static Vector<Complex> MulMatVec(const Matrix<Complex>& a, const Vector<Real>& b) { ... }

static Vector<Complex> MulVecMat(const Vector<Complex>& a, const Matrix<Real>& b) { ... }
static Vector<Complex> MulVecMat(const Vector<Real>& a, const Matrix<Complex>& b) { ... }
```

Example usage

TODO – example with matrices

https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/Chapter_01_basic_objects/demo_matrix.cpp

FUNCTIONS AS FULL-FLEDGED OBJECTS

Function pointers have been in C and C++ from the start.

C++ introduced other options:

- Functors, ie. objects that overload operator()
- Using templates (with use of operator() overloading)
- lambdas

The most general approach is the one taken in Numerical Recipes in C++, where each “function” parameter is actually a template parameter, expecting only implementation of operator().

In an “opinionated” manner of our implementation, we will define a rich set of interfaces and treat functions as full-fledged objects

All interfaces are specified in IFunction.h header

<https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/mml/interfaces/IFunction.h>

General function definition:

```
template<typename _RetType, typename _ArgType>
class IFunction
{
public:
    virtual _RetType operator()(_ArgType) const = 0;
    virtual ~IFunction() {}
};
```

Breaking YAGNI because it is quite hard to envision any kind of function operating only on this interface, but ... you never know.

RealFunction

Interface for real function is simple – real number in, real number out.

```
class IRealFunction : public IFunction<Real, Real>
{
public:
    virtual Real operator()(Real) const = 0;
    virtual ~IRealFunction() {}
};
```

For this interface, we provide two implementations in

<https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/mml/base/Function.h>

First one expects function pointer, meaning it will also accept lambda expression with function definition, giving the user an easy way of creating RealFunction objects:

```

class RealFunction : public IRealFunction
{
    Real(*_func)(const Real);
public:
    RealFunction(Real(*inFunc)(const Real)) : _func(inFunc) {}

    Real operator()(const Real x) const { return _func(x); }
};

```

Second one is initialized with std::function<> object, providing for more complex situations when creating RealFunction objects (for example, when you want to create RealFunction from member function in some class).

```

class RealFunctionFromStdFunc : public IRealFunction
{
    std::function<Real(const Real)> _func;
public:
    RealFunctionFromStdFunc(std::function<Real(const Real)> inFunc) : _func(inFunc) {}

    Real operator()(const Real x) const { return _func(x); }
};

```

Simple example of creating real functions

```

Real already_existing_func(Real x) {
    return sin(x) * (1 + x * x / 2);
}

void Real_functions_case_1_usage()
{
    // creating a function object from an already existing (standalone) function
    RealFunction fReal(already_existing_func);

    // we can also use lambda directly
    RealFunction fReal2( [](Real x) { return sin(x) * (1 + x * x / 2); } );
}

```

More examples, with various capabilities, including using member functions from already existing classes, are given at the end of this section.

ScalarFunction<N>

Representing scalar function that takes vector as an input, and returns real number.

Interface

```

////////////////////////////////////////////////////////////////
template<int N>
class IScalarFunction : public IFunction<Real, const VectorN<Real, N>&>
{
public:
    virtual Real operator()(const VectorN<Real, N>& x) const = 0;

    virtual ~IScalarFunction() {}
};

```

Similarly to RealFunction, it also provides two general implementations of interface.

```
//////////////////////////////////////////////////////////////// SCALAR FUNCTION //////////////////////////////////////////////////////////////////
template<int N>
class ScalarFunction : public IScalarFunction<N>
{
    Real(*_func)(const VectorN<Real, N>&);
public:
    ScalarFunction(Real(*inFunc)(const VectorN<Real, N>&)) : _func(inFunc) {}

    Real operator()(const VectorN<Real, N>& x) const { return _func(x); }
};

template<int N>
class ScalarFunctionFromStdFunc : public IScalarFunction<N>
{
    std::function<Real(const VectorN<Real, N>&)> _func;
public:
    ScalarFunctionFromStdFunc(std::function<Real(const VectorN<Real, N>&)> inFunc) : _func(inFunc) {}

    Real operator()(const VectorN<Real, N>& x) const { return _func(x); }
};
```

VectorFunction<N>

Representing vector function, that returns vector for given vector input parameter.

Interface

```
////////////////////////////////////////////////////////////////
template<int N>
class IVectorFunction : public IFunction<VectorN<Real, N>, const VectorN<Real, N>&>
{
public:
    virtual VectorN<Real, N> operator()(const VectorN<Real, N>& x) const = 0;

    virtual ~IVectorFunction() {}
};
```

Implementations

```
//////////////////////////////////////////////////////////////// VECTOR FUNCTION N -> N //////////////////////////////////////////////////////////////////
template<int N>
class VectorFunction : public IVectorFunction<N>
{
    VectorN<Real, N>(*_func)(const VectorN<Real, N>&);
public:
    VectorFunction(VectorN<Real, N>(*inFunc)(const VectorN<Real, N>&)) : _func(inFunc) {}

    VectorN<Real, N> operator()(const VectorN<Real, N>& x) const { return _func(x); }
};

template<int N>
class VectorFunctionFromStdFunc : public IVectorFunction<N>
{
    std::function<VectorN<Real, N>(const VectorN<Real, N>&)> _func;
public:
    VectorFunctionFromStdFunc(std::function<VectorN<Real, N>(const VectorN<Real, N>&)> inFunc)
        : _func(inFunc) {}

    VectorN<Real, N> operator()(const VectorN<Real, N>& x) const { return _func(x); }
};
```

In similar vein to VectorFunction<N>, we have VectorFunctionNM<N, M>, where input vector is of dimension N, and the function produces vector of different dimension M.

ParametricCurve<N>

Interfaces

Is it really needed to create this additional interface??? Hm ...

```
////////////////////////////////////////////////////////////////
template<int N>
class IRealToVectorFunction : public IFunction<VectorN<Real, N>, Real>
{
public:
    virtual VectorN<Real, N> operator()(Real x) const = 0;

    virtual ~IRealToVectorFunction() {}
};
```

General interface for parametric curve.

```
////////////////////////////////////////////////////////////////
template<int N>
class IParametricCurve : public IRealToVectorFunction<N>
{
public:
    virtual Real getMinT() const = 0;
    virtual Real getMaxT() const = 0;

    std::vector<VectorN<Real, N>> GetTrace(double t1, double t2, int numPoints) const
    {
        std::vector<VectorN<Real, N>> ret;
        double deltaT = (t2 - t1) / (numPoints - 1);
        for (Real t = t1; t <= t2; t += deltaT)
            ret.push_back((*this)(t));
        return ret;
    }

    virtual ~IParametricCurve() {}
};
```

Implementation

```
template<int N>
class ParametricCurve : public IParametricCurve<N>
{
    Real _minT;
    Real _maxT;
    VectorN<Real, N>(*_func)(Real);

public:
    ParametricCurve(VectorN<Real, N>(*inFunc)(Real))
        : _func(inFunc), _minT(Constants::NegativeInf), _maxT(Constants::PositiveInf) {}

    ParametricCurve(Real minT, Real maxT, VectorN<Real, N>(*inFunc)(Real))
        : _func(inFunc), _minT(minT), _maxT(maxT) {}

    Real getMinT() const { return _minT; }
    Real getMaxT() const { return _maxT; }

    virtual VectorN<Real, N> operator()(Real x) const { return _func(x); }
};
```

ParametricSurface<N>

Two different interfaces, for different kinds of surface models.

General surface

```
// complex surface, with fixed u limits, but variable w limits (dependent on u)
template<int N>
class IParametricSurface : public IFunction<VectorN<Real, N>, const VectorN<Real, 2>&>
{
public:
    virtual VectorN<Real, N> operator()(Real u, Real w) const = 0;

    virtual Real getMinU() const = 0;
    virtual Real getMaxU() const = 0;
    virtual Real getMinW(Real u) const = 0;
    virtual Real getMaxW(Real u) const = 0;

    virtual VectorN<Real, N> operator()(const VectorN<Real, 2>& coord) const
    {
        return operator()(coord[0], coord[1]);
    }

    virtual ~IParametricSurface() {}
};
```

Rectangular surface

```
// simple regular surface, defined on rectangular coordinate patch
template<int N>
class IParametricSurfaceRect : public IFunction<VectorN<Real, N>, const VectorN<Real, 2>&>
{
public:
    virtual VectorN<Real, N> operator()(Real u, Real w) const = 0;

    virtual Real getMinU() const = 0;
    virtual Real getMaxU() const = 0;
    virtual Real getMinW() const = 0;
    virtual Real getMaxW() const = 0;

    virtual VectorN<Real, N> operator()(const VectorN<Real, 2>& coord) const
    {
        return operator()(coord[0], coord[1]);
    }

    virtual ~IParametricSurfaceRect() {}
};
```

Example usage

We have five different possibilites for creating function objects.

https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/Chapter_01_basic_objects/demo_functions.cpp

CASE 1 - we already have standalone function providing needed calculation

For example, if we already have a defined set of existing functions:

```
Real Docs_Demo_Functions_RealFunc(Real x) {
| return sin(x) * (1 + x * x / 2);
}

// simple scalar function, returning 1 / r, for given point
Real Docs_Demo_Functions_ScalarFunc(const VectorN<Real>, 3>& x) {
| return 1 / x.NormL2();
}

// little bit more realistic scalar function :
Real Docs_Demo_Functions_Two_Masses_Gravity_Potential(const VectorN<Real>, 3>& x)
{
| const VectorN<Real>, 3> x1{ 10.0, 0.0, 0.0 };
| const VectorN<Real>, 3> x2{ -10.0, 0.0, 0.0 };
| const Real m1 = 1000.0;
| const Real m2 = 1000.0;
| const Real G = 1.0;
| return -G * m1 / (x - x1).NormL2() - G * m2 / (x - x2).NormL2();
}

// TODO - vector function returning field with curl in 2D
VectorN<Real>, 2> Docs_Demo_Functions_VectorFunc(const VectorN<Real>, 2>& x) {
| return VectorN<Real>, 2>{0, x[0] * x[1]};
}

// helix curve in 3D
VectorN<Real>, 3> Docs_Demo_Functions_ParamCurve(Real t) {
| return VectorN<Real>, 3>{ cos(t), sin(t), t};
}

// simple surface
VectorN<Real>, 3> Docs_Demo_Functions_ParamSurface(Real x, Real y) {
| return VectorN<Real>, 3>{x * y, 2 * x * y, 3 * x};
}
```

We can simply create appropriate functions objects by passing function pointers.

```
// creating a function objects from an already existing (standalone) function
RealFunction fReal(Docs_Demo_Functions_RealFunc);
ScalarFunction<3> fScalar(Docs_Demo_Functions_ScalarFunc);
ScalarFunction<3> fScalar2(Docs_Demo_Functions_Two_Masses_Gravity_Potential);
VectorFunction<2> fVector(Docs_Demo_Functions_VectorFunc);
ParametricCurve<3> paramCurve(Docs_Demo_Functions_ParamCurve);
ParametricSurface<3> paramSurface(Docs_Demo_Functions_ParamSurface);
```

CASE 2 - creating function directly from lambda

Extra convenient and useful!

```
RealFunction f2{ [](Real x) { return (Real)sin(x) * (1 + x * x / 2); } };

ScalarFunction<3> fScalar([](const VectorN<Real, 3>& x) { return 1 / x.NormL2(); });
ScalarFunction<3> two_masses_gravity_field_potential{ [](const VectorN<Real, 3>& x)
{
    const VectorN<Real, 3> x1{ 10.0, 0.0, 0.0 };
    const VectorN<Real, 3> x2{ -10.0, 0.0, 0.0 };
    const Real m1 = 1000.0;
    const Real m2 = 1000.0;
    const Real G = 1.0;
    return -G * m1 / (x - x1).NormL2() - G * m2 / (x - x2).NormL2();
}
};

VectorFunction<3> fVector([](const VectorN<Real, 3>& x)
{
    return VectorN<Real, 3>{0, x[0] * x[1], 0};
});

ParametricCurve<3> paramCurve([](Real t) { return VectorN<Real, 3>{t, 2 * t, 3 * t}; });
ParametricSurface<3> paramSurface([](Real x, Real y) { return VectorN<Real, 3>{x * y, 2 * x * y, 3 * x}; });
```

CASE 3 - we have function that has some additional parameters that it depends on (that we might want to vary easily)

We create a class wrapper around that function(ality), and inherit it from appropriate function interface.

```
class TwoMassesGravityPotential : public IScalarFunction<3>
{
    Real _m1, _m2, _G;
    VectorN<Real, 3> _x1, _x2;

public:
    TwoMassesGravityPotential(Real m1, Real m2, Real G,
                             const VectorN<Real, 3>& x1, const VectorN<Real, 3>& x2)
        : _m1(m1), _m2(m2), _G(G), _x1(x1), _x2(x2) {}

    void SetM1(Real m1) { _m1 = m1; }
    void SetM2(Real m2) { _m2 = m2; }
    void SetX1(const VectorN<Real, 3>& x1) { _x1 = x1; }
    void SetX2(const VectorN<Real, 3>& x2) { _x2 = x2; }

    Real operator()(const VectorN<Real, 3>& x) const
    {
        return -_G * (_m1 / (x - _x1).NormL2() + _m2 / (x - _x2).NormL2());
    }
};
```

CASE 4 - there is an already existing external class that has EXACT FUNCTION you want to use (and you can't change the class)

Big class

```
class BigComplexClassYouCantChange1 {
public:
    double _param1, _param2;
    double Weight(double x) const { return 58 * _param1; }

    double UsefulRealFunc(double x) const { return (_param1 * cos(x) + _param2 * sin(x)) / Weight(x); }
};
```

We create RealFunctionFromStdFunc

```
BigComplexClassYouCantChange1 bigObj;

// set parameter values as needed
bigObj._param1 = 1.0;
bigObj._param2 = 2.0;

// declaring f4 as a RealFunction object
RealFunctionFromStdFunc f4(std::function<Real(Real)>{ [&bigObj](Real x)
{
    return bigObj.UsefulRealFunc(x);
}
});
```

And use f4 as normal RealFunction object.

CASE 5 - there is an external class that has data relevant to calculation for your real function, but you can't (or don't want to) change the class.

Class

```
class BigComplexClassYouCantChange2 {
public:
    double _param1, _param2;
    double Weight(double x) const { return 58*_param1; }
};
```

Create a helper class, inherit it from IRealFunction, wrap relevant object with const reference, and use it as RealFunction object wherever it is needed

```
class BigComplexRealFunc2 : public IRealFunction {
    const BigComplexClassYouCantChange2& _ref;
public:
    BigComplexRealFunc2(const BigComplexClassYouCantChange2& bigClass) : _ref(bigClass) { }

    Real operator()(Real x) const {
        return (_ref._param1 * cos(x) + _ref._param2 * sin(x)) / _ref.Weight(x) ;
    }
};
```

Usage

```
BigComplexClassYouCantChange2 bigObj;  
  
bigObj._param1 = 1.0;  
bigObj._param2 = 2.0;  
  
BigComplexRealFunc2    f5(bigObj);      // usable RealFunction object  
  
std::cout << "f5(0.0) = " << f5(0.0) << std::endl;  
std::cout << "f5(1.0) = " << f5(1.0) << std::endl;  
std::cout << "f5(2.0) = " << f5(2.0) << std::endl;
```

CASE 6 - there is an external class that has data relevant to calculation and you need to define multiple real function based on that data

TODO - Show examples of creating different kinds of:

- real function objects
- scalar function objects
- vector functions objects
- parametric curves
- parametric surfaces

BASIC GEOMETRY IN 2D AND 3D

Defining objects that will represent concepts from 2D and 3D analytical geometry – points, vectors, lines, planes.

Points

Why special classes for points, when they are structurally same as vectors, and position is mostly defined as “radius vector”? In authors opinion, semantics is important, and type system should be utilized to support it.

Example, Cartesian point in 3D

Mostly trivial and expected operations for a point:

<https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/mml/base/Geometry.h>

```
class Point3Cartesian
{
private:
    Real _x, _y, _z;

public:
    Real X() const { return _x; }
    Real& X() { return _x; }
    Real Y() const { return _y; }
    Real& Y() { return _y; }
    Real Z() const { return _z; }
    Real& Z() { return _z; }

    Point3Cartesian() : _x(0), _y(0), _z(0) {}
    Point3Cartesian(Real x, Real y, Real z) : _x(x), _y(y), _z(z) {}

    Real Dist(const Point3Cartesian& b) const { ... }

    bool operator==(const Point3Cartesian& b) const { ... }
    bool operator!=(const Point3Cartesian& b) const { ... }

    Point3Cartesian operator+(const Point3Cartesian& b) const { ... }
    Point3Cartesian operator*(Real b) { ... }
    Point3Cartesian operator/(Real b) { ... }

    friend Point3Cartesian operator*(Real a, const Point3Cartesian& b) { ... }
};
```

There's a question of semantic validity of operator+() in this class, where adding two points is, even though mathematically precisely defined, something that looks off - namely, if you want to “add” to point, that is something you would do with a vector.

However, “adding” points is essential when we want to find middle points of a segment line or centroid of a triangle, and also for doing any kind of interpolation between two points, so it is part of the interface.

Vectors

Vector is NOT a point!

Point denotes position in space, in given coordinate system, vectors are ... well, much more complex beasts

Cartesian vectors are simplest, as they are examples of *free vectors*, which are the same at every position in space, meaning that their component representation doesn't depend on position, unlike, for example vectors in spherical coordinate system.

We will deal with position-dependent kinds of vectors in Chapter 10 – Coordinate transformations, and for now cartesian vectors will do.

Example of Vector3Cartesian:

Specialized from VectorN, with Real type and dimension 3.

<https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/mml/base/VectorTypes.h>

```
class Vector3Cartesian : public VectorN<Real, 3>
{
public:
    Real X() const { return _val[0]; }
    Real& X() { return _val[0]; }
    Real Y() const { return _val[1]; }
    Real& Y() { return _val[1]; }
    Real Z() const { return _val[2]; }
    Real& Z() { return _val[2]; }

    Vector3Cartesian() : VectorN<Real, 3>{ 0.0, 0.0, 0.0 } {}
    Vector3Cartesian(const VectorN<Real, 3>& b) : VectorN<Real, 3>{ b } {}
    Vector3Cartesian(Real x, Real y, Real z) : VectorN<Real, 3>{ x, y, z } {}
    Vector3Cartesian(std::initializer_list<Real> list) : VectorN<Real, 3>(list) {}
    Vector3Cartesian(const Point3Cartesian& a, const Point3Cartesian& b) { ... }

    Point3Cartesian getAsPoint() { ... }
```

Set of arithmetic operations

```
Point3Cartesian getAsPoint() { ... }

// For Cartesian vector, we will enable operator* to represent standard scalar product
Real operator*(const Vector3Cartesian& b) const { ... }

friend Vector3Cartesian operator*(const Vector3Cartesian& a, Real b) { ... }
friend Vector3Cartesian operator*(Real a, const Vector3Cartesian& b) { ... }
friend Vector3Cartesian operator/(const Vector3Cartesian& a, Real b) { ... }

friend Vector3Cartesian operator-(const Point3Cartesian& a, const Point3Cartesian& b)

friend Point3Cartesian operator+(const Point3Cartesian& a, const Vector3Cartesian& b)
friend Point3Cartesian operator-(const Point3Cartesian& a, const Vector3Cartesian& b)
```

And some more

```
bool IsParallelTo(const Vector3Cartesian& b, Real eps = 1e-15) const { ... }
bool IsPerpendicularTo(const Vector3Cartesian& b, Real eps = 1e-15) const { ... }
Real AngleToVector(const Vector3Cartesian& b) { ... }

friend Real ScalarProduct(const Vector3Cartesian& a, const Vector3Cartesian& b) { ... }
friend Vector3Cartesian VectorProd(const Vector3Cartesian& a, const Vector3Cartesian& b)
```

Lines

There are multiple ways of defining lines (TODO)

In our case, in both 2D and 3D cases they are specified with point, and vector representing direction, ie. representing parametric line equation.

Example Line3D

<https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/mml/base/Geometry3D.h>

```
class Line3D
{
private:
    Point3Cartesian _point;
    Vector3Cartesian _direction;

public:
    Line3D() {}
    // by default, direction vector is normalized to unit vector (but, it need not be such!)
    Line3D(const Point3Cartesian& pnt, const Vector3Cartesian dir) { ... }
    Line3D(const Point3Cartesian& a, const Point3Cartesian& b) { ... }

    Point3Cartesian StartPoint() const { return _point; }
    Point3Cartesian& StartPoint() { return _point; }

    Vector3Cartesian Direction() const { return _direction; }
    Vector3Cartesian& Direction() { return _direction; }

    Point3Cartesian operator()(Real t) const { return _point + t * _direction; }

    bool IsPerpendicular(const Line3D& b) const { ... }
    bool IsParallel(const Line3D& b) const { ... }
```

More operations:

```
// distance between point and line
Real Dist(const Point3Cartesian& pnt) const { ... }

// distance between two lines
Real Dist(const Line3D& line) const { ... }
// distance between two lines, while also returning nearest points on both lines
Real Dist(const Line3D& line, Point3Cartesian& out_line1_pnt, Point3Cartesian& out_line2_pnt) const { ... }

// nearest point on line to given point
Point3Cartesian NearestPointOnLine(const Point3Cartesian& pnt) const { ... }

// intersection of two lines
bool Intersection(const Line3D& line, Point3Cartesian& out_inter_pnt) const { ... }

// perpendicular line that goes through given point
Line3D PerpendicularLineThroughPoint(const Point3Cartesian& pnt) { ... }
```

Polygons

BIG TODO!!!!

```
class Polygon2D
{
private:
    std::vector<Point2Cartesian> _points;
public:
    Polygon2D() {}
    Polygon2D(std::vector<Point2Cartesian> points) : _points(points) {}
    Polygon2D(std::initializer_list<Point2Cartesian> list) { ... }

    std::vector<Point2Cartesian> Points() const { return _points; }
    std::vector<Point2Cartesian>& Points() { return _points; }

    Real Area() const { ... }

    bool IsSimple() const { ... }

    bool IsConvex() const { ... }

    std::vector<Triangle2D> Triangularization() const { ... }

    bool IsInside(Point2Cartesian pnt) const { ... }
};
```

Plane3D class

Representing plane in 3D Cartesian space, with general equation $Ax + By + Cz + D = 0$.

Extensive set of constructors,

```
class Plane3D
{
private:
    Real _A, _B, _C, _D;

public:
    Plane3D(const Point3Cartesian& a, const Vector3Cartesian& normal) { ... }
    Plane3D(const Point3Cartesian& a, const Point3Cartesian& b, const Point3Cartesian& c) { ... }
    // Hesse normal form
    Plane3D(Real alpha, Real beta, Real gamma, Real d) { ... }
    // segments on coordinate axes
    Plane3D(Real seg_x, Real seg_y, Real seg_z) { ... }

    static Plane3D GetXYPlane() { return Plane3D(Point3Cartesian(0, 0, 0), Vector3Cartesian(0, 0, 1)); }
    static Plane3D GetXZPlane() { return Plane3D(Point3Cartesian(0, 0, 0), Vector3Cartesian(0, 1, 0)); }
    static Plane3D GetYZPlane() { return Plane3D(Point3Cartesian(0, 0, 0), Vector3Cartesian(1, 0, 0)); }

    Real A() const { return _A; }
    Real& A() { return _A; }
    Real B() const { return _B; }
    Real& B() { return _B; }
    Real C() const { return _C; }
    Real& C() { return _C; }
    Real D() const { return _D; }
    Real& D() { return _D; }

    Vector3Cartesian Normal() const { return Vector3Cartesian(_A, _B, _C); }
    Point3Cartesian GetPointOnPlane() const { ... }

    void GetCoordAxisSegments(Real& outseg_x, Real& outseg_y, Real& outseg_z) { ... }
```

Basic operations between plane and points, lines, and other planes.

```
// point to plane operations
bool IsPointOnPlane(const Point3Cartesian& pnt, Real defEps = 1e-15) const { ... }
Real DistToPoint(const Point3Cartesian& pnt) const { ... }

Point3Cartesian ProjectionToPlane(const Point3Cartesian& pnt) const { ... }

// line to plane operations
bool IsLineOnPlane(const Line3D& line) const { ... }
Real AngleToLine(const Line3D& line) const { ... }
bool IntersectionWithLine(const Line3D& line, Point3Cartesian& out_inter_pnt) const { ... }

// plane to plane operations
bool IsParallelToPlane(const Plane3D& plane) const { ... }
bool IsPerpendicularToPlane(const Plane3D& plane) const { ... }
Real AngleToPlane(const Plane3D& plane) const { ... }
Real DistToPlane(const Plane3D& plane) const { ... }
bool IntersectionWithPlane(const Plane3D& plane, Line3D& out_inter_line) const { ... }
```

Triangles

Each triangle has A(), B(), C() member functions ... but not enforced through interface!

Basic (geometrical) triangle.

```
class Triangle
{
private:
    Real _a, _b, _c;

public:
    Real A() const { return _a; }
    Real& A() { return _a; }
    Real B() const { return _b; }
    Real& B() { return _b; }
    Real C() const { return _c; }
    Real& C() { return _c; }

    Triangle() : _a(0.0), _b(0.0), _c(0.0){}
    Triangle(Real a, Real b, Real c) : _a(a), _b(b), _c(c) {}

    Real Area() const { ... }

    bool IsRight() const { ... }
    bool IsIsosceles() const { ... }
    bool IsEquilateral() const { ... }
};
```

Triangle in 2D plane

```
class Triangle2D
{
private:
    Point2Cartesian _pnt1, _pnt2, _pnt3;

public:
    Triangle2D(Point2Cartesian pnt1, Point2Cartesian pnt2, Point2Cartesian pnt3)

    Real A() const { return _pnt1.Dist(_pnt2); }
    Real B() const { return _pnt2.Dist(_pnt3); }
    Real C() const { return _pnt3.Dist(_pnt1); }

    Point2Cartesian Pnt1() const { return _pnt1; }
    Point2Cartesian& Pnt1() { return _pnt1; }
    Point2Cartesian Pnt2() const { return _pnt2; }
    Point2Cartesian& Pnt2() { return _pnt2; }
    Point2Cartesian Pnt3() const { return _pnt3; }
    Point2Cartesian& Pnt3() { return _pnt3; }

    Real Area() const { ... }
};
```

Triangle in 3D space

```
class Triangle3D
{
protected:
    Point3Cartesian _pnt1, _pnt2, _pnt3;
public:
    Triangle3D() {}
    Triangle3D(Point3Cartesian pnt1, Point3Cartesian pnt2, Point3Cartesian pnt3) { ... }

    Real A() const { return _pnt1.Dist(_pnt2); }
    Real B() const { return _pnt2.Dist(_pnt3); }
    Real C() const { return _pnt3.Dist(_pnt1); }

    Point3Cartesian Pnt1() const { return _pnt1; }
    Point3Cartesian& Pnt1() { return _pnt1; }
    Point3Cartesian Pnt2() const { return _pnt2; }
    Point3Cartesian& Pnt2() { return _pnt2; }
    Point3Cartesian Pnt3() const { return _pnt3; }
    Point3Cartesian& Pnt3() { return _pnt3; }

    Real Area() const { ... }

    bool IsRight() const { ... }
    bool IsIsosceles() const { ... }
    bool IsEquilateral() const { ... }

    Plane3D getDefinedPlane() const { ... }
};
```

Making Triangle3D a ParametricSurface<3>

So it can be used in surface integration routines!

```

// Represents triangular surface in 3D and defines all needed mappings
// to represent Triangle3D as IParametricSurface
class TriangleSurface3D : public Triangle3D, IParametricSurface<3>
{
public:
    Real _minX, _maxX, _minY, _maxY;
    Point3Cartesian _origin;
    Point3Cartesian _center;
    Vector3Cartesian _localX, _localY;
    Vector3Cartesian _normal;
    Real _pnt3XCoord;

    // pnt1-pnt2 should be hypotenuse of the triangle!!!
    // but we will handle it, if it is not
    TriangleSurface3D(Point3Cartesian pnt1, Point3Cartesian pnt2, Point3Cartesian pnt3) { ... }

    virtual Real getMinU() const { return _minX; }
    virtual Real getMaxU() const { return _maxX; }
    virtual Real getMinW(Real u) const { return _minY; }
    virtual Real getMaxW(Real u) const { ... }

    // for a given (u,w), which is basically (x,y) in local coordinate system
    // return point in global coordinate system
    VectorN<Real, 3> operator()(Real u, Real w) const { ... }
};


```

Boxes

TODO!

Modeling surfaces & solid bodies

Two approaches

- Boundaries defined by functions
- Composed of surface polygons that (hopefully) enclose the body

Example usage - geometry

Analytical geometry examples in 2d and 3d

Creating bodies

https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/Chapter_01_basic_objects/demo_geometry.cpp

2. Visualization, anyone?

USING QT

Ideal for open-source projects

Widgets, enabling interactive application

2D animation for collision simulator

Creating simple application for visualization of moving circles within given rectangle.

We will be extending this in Chapter 4, for collision simulator.

USING FLTK

Simple to use, and cross-platform, FLTK is another option, especially if Qt open source (or commercial) license is not suitable.

Visualizing real function

Short example of visualizing real function in some interval.

USING PYTHON – MATHPLOTLIB BINDING

Matplotlib is beautiful piece of software, and by creating interface between our C++ code and Python, we can efficiently utilize it.

Based on book “Introduction to numerical programming” by Titus Adrian Beu and toolkit presented there.

Contour plot

USING VTK?

To do, or not to do?

It is cross-platform, and powerful in its visualization capabilities

USING .NET WPF ON WINDOWS

Unlike previous visualization solutions, this one is available only for Windows, as it relies on mighty Windows Presentation Foundation framework for visualization.

It is similar in its usage pattern to GnuPlot where we need to export all relevant data that needs visualizing in a file, and then give that file as an input to WPF visualizing application.

WPF visualizers are realized as a set of distinct applications, with each one of them focusing on one type of visualization. So far, following visualizations are available:

- 1) RealFunctionVisualizer (with capability of visualizing multiple functions)
- 2) ScalarFunction2DVisualizer – for visualizing 2D surfaces given as $z=f(x,y)$ on rectangular patch
- 3) ParametricCurve2DVisualizer
- 4) ParametricCurve3DVisualizer
- 5) VectorField2DVisualizer – for visualizing vector field in 2D
- 6) VectorField3DVisualizer – for
- 7) ParticleVisualizer2D
- 8) ParticleVisualizer3D

Helper Serializer class

To relieve user of manually creating input files for given visualizers, Serializer class was created, with a extensive set of static functions for writing to files different kind of data.

Functionality for serializing real functions.

```
// Real function serialization
// serializing values at equally spaced points in given interval
static bool SaveRealFunc(const IRealFunction& f, std::string title,
    Real x1, Real x2, int numPoints, std::string fileName) { ... }

// serializing values at given list of points
static bool SaveRealFunc(const IRealFunction& f, std::string title,
    Vector<Real> points, std::string fileName) { ... }

// serializing multiple functions in a single files
static bool SaveRealMultiFunc(std::vector<IRealFunction*> funcs, std::string title,
    Real x1, Real x2, int numPoints, std::string fileName) { ... }

// same as SaveRealFunc, but points are not explicitly written in file
// (as they can be calculated from x1, x2 and numPoints)
static bool SaveRealFuncEquallySpaced(const IRealFunction& f, std::string title,
    Real x1, Real x2, int numPoints, std::string fileName)
```

Parametric curves

```
// Parametric curve serialization
template<int N>
static bool SaveParamCurve(const IRealToVectorFunction<N>& f, std::string inType, std::string title,
    Real t1, Real t2, int numPoints, std::string fileName) { ... }

template<int N>
static bool SaveParamCurve(const IRealToVectorFunction<N>& f, std::string inType, std::string title,
    Vector<Real> points, std::string fileName) { ... }

template<int N>
static bool SaveAsParamCurve(std::vector<VectorN<Real, N>> vals, std::string inType, std::string title,
    Real t1, Real t2, int numPoints, std::string fileName) { ... }

static bool SaveAsParamCurve2D(Vector<Real> vec_x, Vector<Real> vec_y) { ... }

// Helper/forwarding functions
static bool SaveParamCurveCartesian2D(const IRealToVectorFunction<2>& f, std::string title,
    Real t1, Real t2, int numPoints, std::string fileName) { ... }

static bool SaveParamCurveCartesian3D(const IRealToVectorFunction<3>& f, std::string title,
    Real t1, Real t2, int numPoints, std::string fileName) { ... }
```

Scalar function serialization

```
// Scalar function serialization
static bool SaveScalarFunc2DCartesian(const IScalarFunction<2>& f, std::string title,
    Real x1, Real x2, int numPointsX,
    Real y1, Real y2, int numPointsY, std::string fileName)

static bool SaveScalarFunc3DCartesian(const IScalarFunction<3>& f, std::string title,
    Real x1, Real x2, int numPointsX,
    Real y1, Real y2, int numPointsY,
    Real z1, Real z2, int numPointsZ, std::string fileName)
```

Vector function serialization

2D versions

```
// 2D vector function serialization
static bool SaveVectorFunc2D( const IVectorFunction<2>& f, std::string inType, std::string title,
                           Real x1_start, Real x1_end, int numPointsX1,
                           Real x2_start, Real x2_end, int numPointsX2, std::string fileName)[]

static bool SaveVectorFunc2D( const IVectorFunction<2>& f, std::string inType, std::string title,
                           Real x1_start, Real x1_end, int numPointsX1,
                           Real x2_start, Real x2_end, int numPointsX2,
                           std::string fileName, Real upper_threshold) { ... }

static bool SaveVectorFunc2DCartesian(const IVectorFunction<2>& f, std::string title,
                                      Real x1, Real x2, int numPointsX,
                                      Real y1, Real y2, int numPointsY, std::string fileName) { . .

static bool SaveVectorFunc2DCartesian(const IVectorFunction<2>& f, std::string title,
                                      Real x1, Real x2, int numPointsX,
                                      Real y1, Real y2, int numPointsY, std::string fileName,
                                      Real upper_threshold) { ... }
```

And 3D versions

```
// 3D vector function serialization
static bool SaveVectorFunc3D(const IVectorFunction<3>& f, std::string inType, std::string title,
                           Real x1_start, Real x1_end, int numPointsX1,
                           Real x2_start, Real x2_end, int numPointsX2,
                           Real x3_start, Real x3_end, int numPointsX3, std::string fileName)[]

static bool SaveVectorFunc3D(const IVectorFunction<3>& f, std::string inType, std::string title,
                           Real x1_start, Real x1_end, int numPointsX1,
                           Real x2_start, Real x2_end, int numPointsX2,
                           Real x3_start, Real x3_end, int numPointsX3,
                           std::string fileName, Real upper_threshold) { ... }

static bool SaveVectorFunc3DCartesian(const IVectorFunction<3>& f, std::string title,
                                      Real x1, Real x2, int numPointsX,
                                      Real y1, Real y2, int numPointsY,
                                      Real z1, Real z2, int numPointsZ, std::string fileName) { .
static bool SaveVectorFunc3DCartesian(const IVectorFunction<3>& f, std::string title,
                                      Real x1, Real x2, int numPointsX,
                                      Real y1, Real y2, int numPointsY,
                                      Real z1, Real z2, int numPointsZ, std::string fileName,
                                      Real upper_threshold) { ... }
```

Particle simulation serializers

```
// particle simulation serialization
static bool SaveParticleSimulation2D(std::string fileName, int numBalls,
                                     std::vector<std::vector<Pnt2Cart>> ballPositions,
                                     std::vector<std::string> ballColors, std::vector<double> ballRadius )

static bool SaveParticleSimulation3D(std::string fileName, int numBalls,
                                     std::vector<std::vector<Pnt3Cart>> ballPositions,
                                     std::vector<std::string> ballColors, std::vector<double> ballRadius)[]
```

ODE solution serializers

```
// ODESolution serialization
static bool SaveODESolutionAsMultiFunc(const ODESystemSolution& sol, std::string title, std::string fileName)

static bool SaveODESolAsParametricCurve2D(const ODESystemSolution& sol, std::string fileName,
                                         int ind1, int ind2, std::string title) { ... }

static bool SaveODESolAsParametricCurve3D(const ODESystemSolution& sol, std::string fileName,
                                         int ind1, int ind2, int ind3, std::string title) { ... }
```

Helper Visualizer class

- All WPF visualizers are distinct applications, so from our console applications they have to be started with appropriate parameters, ie. Names of input files
- Serializer helps in creating those files,
- Visualizer ties it all together

We are starting with a set of paths:

```
class Visualizer
{
    static inline std::string _pathResultFiles{ MML_PATH_ResultFiles };

    static inline std::string _pathRealFuncViz{ MML_PATH_RealFuncViz };
    static inline std::string _pathSurfaceViz{ MML_PATH_SurfaceViz };
    static inline std::string _pathParametricCurve3DViz{ MML_PATH_ParametricCurve3DViz };
    static inline std::string _pathParametricCurve2DViz{ MML_PATH_ParametricCurve2DViz };
    static inline std::string _pathVectorField2DViz{ MML_PATH_VectorField2DViz };
    static inline std::string _pathVectorField3DViz{ MML_PATH_VectorField3DViz };

    static inline std::string _pathParticle2DViz{ MML_PATH_Particle2DViz };
    static inline std::string _pathParticle3DViz{ MML_PATH_Particle3DViz };
```

Set of visualizers for real functions

```
// visualizations of Real function
static void VisualizeRealFunction(const IRealFunction& f, std::string title,
                                  Real x1, Real x2, int numPoints, std::string fileName) { .. }

static void VisualizeRealFunction(const IRealFunction& f, std::string title,
                                  Vector<Real> points, std::string fileName) { ... }

static void VisualizeMultiRealFunction(std::vector<IRealFunction*> funcs, std::string title,
                                       std::vector<std::string> func_legend,
                                       Real x1, Real x2, int numPoints, std::string fileName)
```

Visualization for scalar function in 2D.

```

// visualizations of Scalar function in 2D
static void VisualizeScalarFunc2DCartesian(const IScalarFunction<2>& func, std::string title,
                                            Real x1, Real x2, int numPointsX,
                                            Real y1, Real y2, int numPointsY, std::string fileName)

```

Visualizations for vector fields

```

// visualizations of Vector fields
static void VisualizeVectorField2DCartesian(const IVectorFunction<2>& func, std::string title,
                                             Real x1, Real x2, int numPointsX,
                                             Real y1, Real y2, int numPointsY, std::string fileName)

static void VisualizeVectorField3DCartesian(const IVectorFunction<3>& func, std::string title,
                                            Real x1, Real x2, int numPointsX,
                                            Real y1, Real y2, int numPointsY,
                                            Real z1, Real z2, int numPointsZ, std::string fileName)

```

Parametric curves have extensive support for visualization.

```

static void VisualizeParamCurve2D(const IRealToVectorFunction<2>& f, std::string title,
                                  Real t1, Real t2, int numPoints,
                                  std::string fileName) { ... }

static void VisualizeMultiParamCurve2D(std::vector<IRealToVectorFunction<2>> curves,
                                       std::string title,
                                       Real t1, Real t2,
                                       int numPoints, std::string fileName) { ... }

static void VisualizeParamCurve3D(const IRealToVectorFunction<3>& f, std::string title,
                                  Real t1, Real t2, int numPoints,
                                  std::string fileName) { ... }

static void VisualizeMultiParamCurve3D(std::vector<IRealToVectorFunction<3>> curves,
                                       std::string title,
                                       Real t1, Real t2, int numPoints,
                                       std::string fileName) { ... }

static void VisualizeMultiParamCurve3D(std::vector<std::string> fileNames) { ... }

```

ODE system solution visualizations.

```

// ODE Solution visualizations
static void VisualizeODESysSolAsMultiFunc(const ODESysSolution& sol,
                                           std::string title, std::string fileName) {}

static void VisualizeODESysSolAsParamCurve2(const ODESysSolution& sol,
                                             int ind1, int ind2,
                                             std::string title, std::string fileName) {}

static void VisualizeODESysSolAsParamCurve3(const ODESysSolution& sol,
                                             int ind1, int ind2, int ind3,
                                             std::string title, std::string fileName) {}

static void VisualizeODESysSolAsParamCurve3(const ODESysSolution& sol,
                                             std::string title, std::string fileName) { ... }

```

Example how it is mostly done in all functions (basically, it uses existing Serializer object that can serialize to a file value for different kinds of functions, and then, using defined paths for visualizers, creates system command to call them with appropriate parameters):

```
static void VisualizeRealFunction(const IRealFunction& f, std::string title,
                                  Real x1, Real x2, int numPoints, std::string fileName)
{
    std::string name = _pathResultFiles + fileName;
    Serializer::SaveRealFunc(f, title, x1, x2, numPoints, name);

#if defined(MML_PLATFORM_WINDOWS)
    std::string command = _pathRealFuncViz + " " + name;
    system(command.c_str());
#else
    std::cout << "VisualizeRealFunction: Not implemented for this OS" << std::endl;
#endif
}
```

Visualizing real functions

RealFunctionVisualizer is implemented as a .NET Core 8 WPF application.

Simple structure – it loads all given input files, does necessary analysis of ranges and values, and then visualizes all data on a WPF Canvas.

Supported input types:

REAL_FUNCTION

Visualizing real function is quite simple:

```
RealFunction f1{ [](Real x) { return sin(x) * (x - 3) * (x + 5) / exp(0.2 / std::abs(2 - x)); } };

Visualizer::VisualizeRealFunction(f1, "Simple function", -10.0, 10.0, 501,
                                "example3_wpf_real_func1.txt");
```

File “example3_wpf_real_func.txt” has following format:

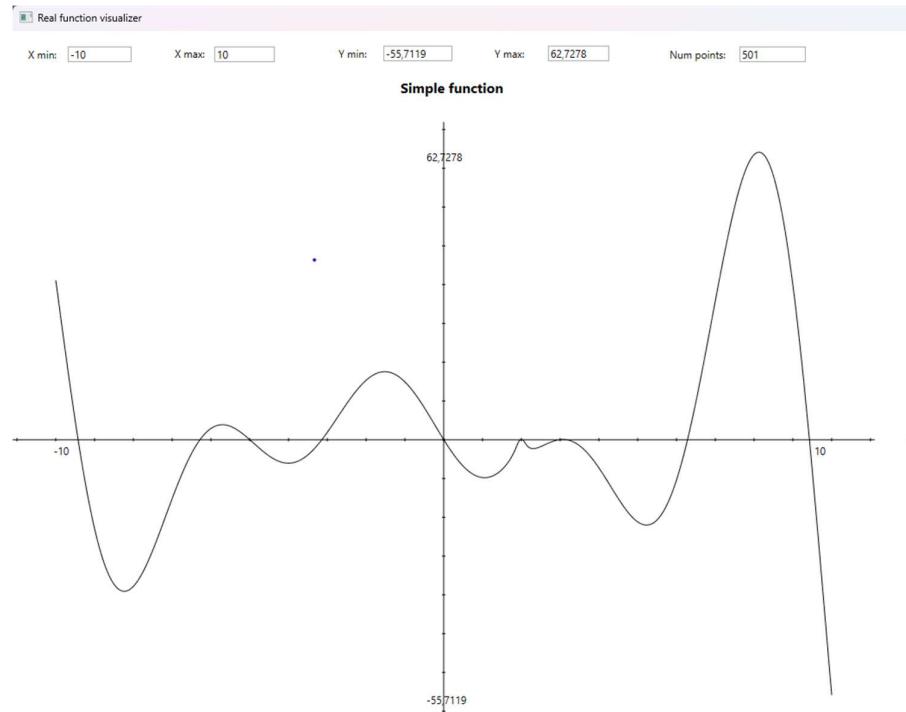
```
REAL_FUNCTION
Simple function
x1: -10
x2: 10
NumPoints: 501
-10 34.7769
-9.96 32.242
-9.92 29.7058
-9.88 27.1733
-9.84 24.6492
-9.8 22.1381
...
9.8 -35.9488
9.84 -39.9153
```

```

9.88 -43.8821
9.92 -47.842
9.96 -51.7877
10 -55.7119

```

And we get following visualization:



We can easily calculate and then visualize function derivation (and show both together).

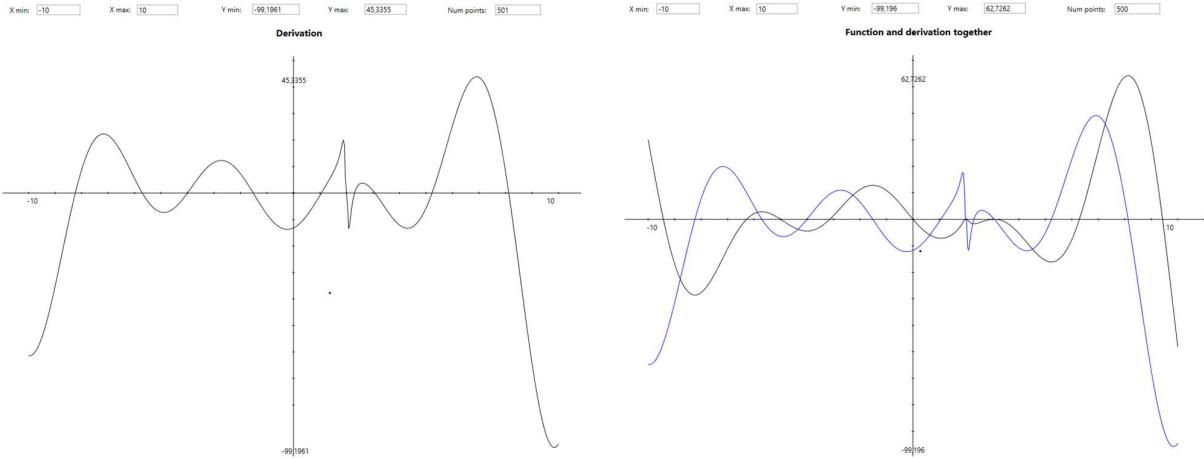
```

RealFuncDerived4 f1_der;           // 4th order derivation of f1 function

Visualizer::VisualizeRealFunction(f1_der, "Derivation", -10.0, 10.0, 501,
                                  "example3_wpf_real_func2.txt");

// shown together
Visualizer::VisualizeMultiRealFunction({ &f1, &f1_der }, "Function and derivation together",
                                       -10.0, 10.0, 501, "example3_wpf_multi_real_func.txt");

```



REAL_FUNCTION_EQUALLY_SPACED

Similar, but has only one value in a row since 'x' value is calculated from x1, x2 and NumPoints parameters.

Use if you need to save on file size.

MULTI_REAL_FUNCTION

In previous example we've seen how we can visualize real functions when we have different object representing them, but one other important usage is for visualizing solutions of differential equations.

Solving Lorentz system is simple (OK, we are getting a little bit ahead of ourselves):

```
// Solving Lorentz system as MULTI_REAL_FUNCTION example
ODESystem lorentz_system(3, [] (Real t, const Vector<Real>& x, Vector<Real>& dxdt)
{
    const Real sigma = 10.0;
    const Real rho = 28.0;
    const Real beta = 8.0 / 3.0;
    dxdt[0] = sigma * (x[1] - x[0]);
    dxdt[1] = x[0] * (rho - x[2]) - x[1];
    dxdt[2] = x[0] * x[1] - beta * x[2];
};

Vector<Real> ystart({ 2.0, 1.0, 1.0 });
ODESystemSolver<RK5_CashKarp_Stepper> solver(lorentz_system);
ODESystemSolution sol = solver.integrate(ystart, 0.0, 50.0, 0.1, 1e-08, 0.01);

Visualizer::VisualizeODESysSolAsMultiFunc(sol, "Lorentz system", "example3_wpf_lorentz.txt");
```

We get following data in file (parameters at the beginning are: graph title, number of functions (expected number of values in the row), x1, x2 and number of points).

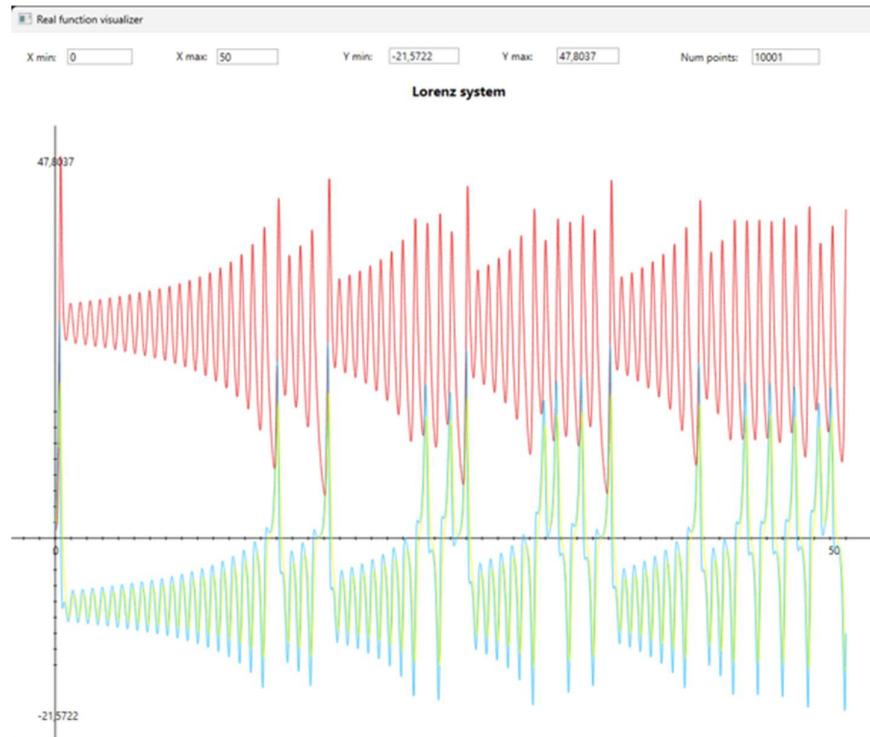
```
MULTI_REAL_FUNCTION
Lorentz system
3
```

```

x1: 0
x2: 50
NumPoints: 478
0 2 1 1
0.108108 3.65659 7.54213 1.7794
0.209965 10.8358 21.4095 10.6551
0.314271 19.4985 17.8098 44.4869
0.416696 6.86177 -7.84692 38.1623
0.517103 -2.91685 -8.29004 28.4874
0.620594 -6.26595 -8.2665 25.2455
...
49.4665 3.54238 -2.88674 30.0554
49.5697 -0.504479 -2.62469 22.5465
49.6769 -2.1692 -3.61403 17.3492
49.7775 -4.14473 -6.89177 14.7035
49.8823 -8.39311 -13.8369 17.0854
49.9881 -14.0495 -17.2098 30.9598
50 -14.3586 -16.3486 32.7962

```

And the following visualization.



Visualizing parametric curves in 2D and 3D

Parametric curves in 2D

We'll be using predefined curves.

Starting with lemniscate.

```

LemniscateCurve lemniscate;
Visualizer::VisualizeParamCurve2D(lemniscate, "Lemniscate", 0.0, 2 * Constants::PI, 101,
                                "example3_wpf_curve_lemniscate.txt");

```

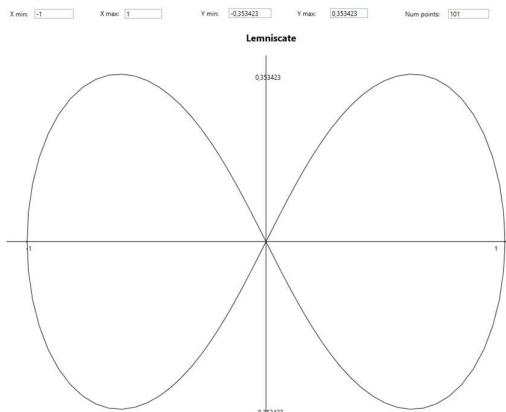
Generated file:

```

PARAMETRIC_CURVE_CARTESIAN_2D
Lemniscate
t1: 0
t2: 6.28319
NumPoints: 101
0 1 0
0.0628319 0.994107 0.0624205
0.125664 0.976771 0.122422
0.188496 0.948967 0.177819
0.251327 0.912169 0.226847
0.314159 0.868155 0.268275
...
5.96903 0.868155 -0.268275
6.03186 0.912169 -0.226847
6.09469 0.948967 -0.177819
6.15752 0.976771 -0.122422
6.22035 0.994107 -0.0624205
6.28319 1 -9.12671e-15

```

And visualization.



Log spiral curve

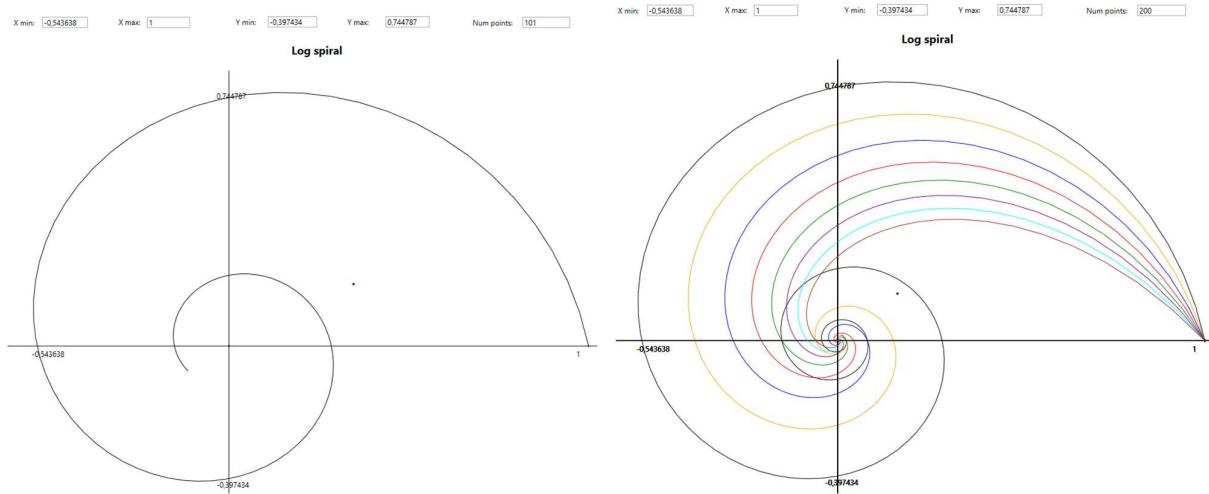
```

LogSpiralCurve log_spiral2(-0.2), log_spiral3(-0.3), log_spiral4(-0.4), log_spiral5(-0.5), log_spiral6(-0.6);
LogSpiralCurve log_spiral7(-0.7), log_spiral8(-0.8), log_spiral9(-0.9);

Visualizer::VisualizeParamCurve2D(log_spiral2, "Log spiral", 0.0, 10.0, 101,
                                "example3_wpf_curve_log_spiral.txt");

Visualizer::VisualizeMultiParamCurve2D({ &log_spiral2, &log_spiral3, &log_spiral4, &log_spiral5,
                                         &log_spiral6, &log_spiral7, &log_spiral8, &log_spiral9 },
                                         "Log spiral", 0.0, 20.0, 201, "example3_wpf_curve_log_spiral_multi");

```

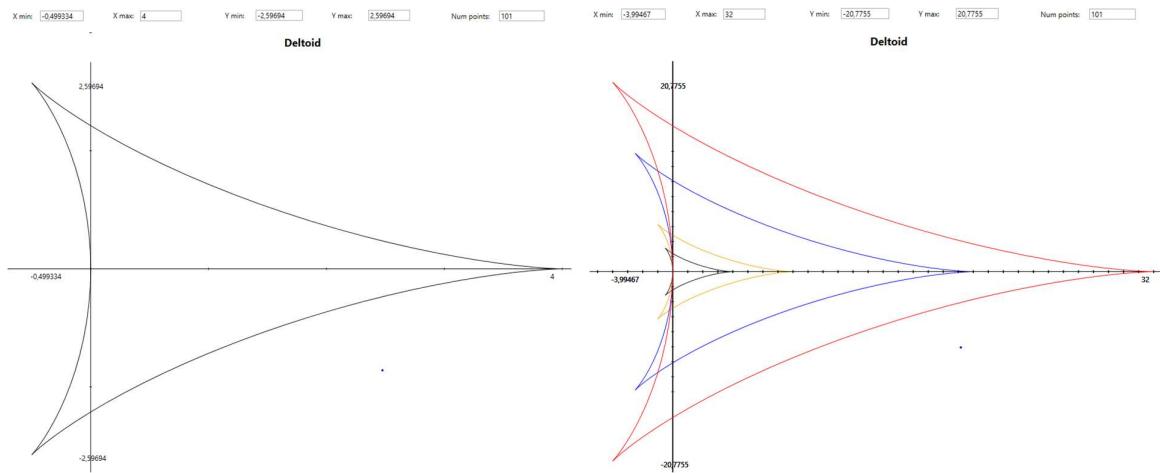


Deltoid

```
DeltoidCurve deltoid1(1), deltoid2(2), deltoid3(5), deltoid4(8), deltoid5(10), deltoid6(15);

Visualizer::VisualizeParamCurve2D(deltoid1, "Deltoid", 0.0, 2 * Constants::PI, 101,
                                  "example3_wpf_curve_deltoid.txt");

Visualizer::VisualizeMultiParamCurve2D({ &deltoid1, &deltoid2, &deltoid3, &deltoid4 },
                                       "Deltoid", 0.0, 2 * Constants::PI, 101,
                                       "example3_wpf_curve_deltoid_multi");
```



Astroid

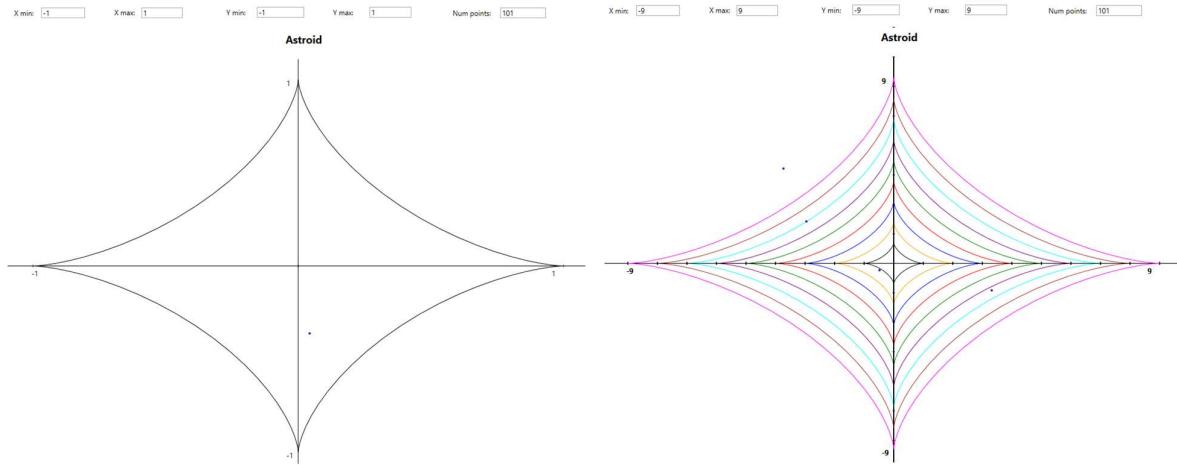
```

AstroidCurve astroid1(1), astroid2(2.0), astroid3(3.0), astroid4(4.0);
AstroidCurve astroid5(5.0), astroid6(6.0), astroid7(7.0), astroid8(8.0), astroid9(9.0);

Visualizer::VisualizeParamCurve2D(astroid1, "Astroid", 0.0, 2 * Constants::PI, 101,
                                    "example3_wpf_curve_astroid.txt");

Visualizer::VisualizeMultiParamCurve2D({ &astroid1, &astroid2, &astroid3, &astroid4, &astroid5,
                                         &astroid6, &astroid7, &astroid8, &astroid9 },
                                         "Astroid", 0.0, 2 * Constants::PI, 101,
                                         "example3_wpf_curve_astroid_multi");

```



Parametric curves in 3D

```

// using predefined 3D curves for visualization example
HelixCurve      helix(20.0, 2.0);
ToroidalSpiralCurve toroid1(5, 20.0), toroid2(5, 10.0), toroid3(5, 5.0);

Visualizer::VisualizeParamCurve3D(helix, "helix", -50.0, 50.0, 1000,
                                    "example3_wpf_curve_helix.txt");

Visualizer::VisualizeParamCurve3D(toroid1, "toroid", 0.0, 5 * Constants::PI, 1000,
                                    "example3_wpf_curve_toroid.txt");

// visualize all three curves
Visualizer::VisualizeMultiParamCurve3D({ &toroid1, &toroid2, &toroid3 }, "toroidal spiral",
                                         0.0, 5 * Constants::PI, 1000,
                                         "example3_wpf_curve_toroidal_spiral.txt");

```

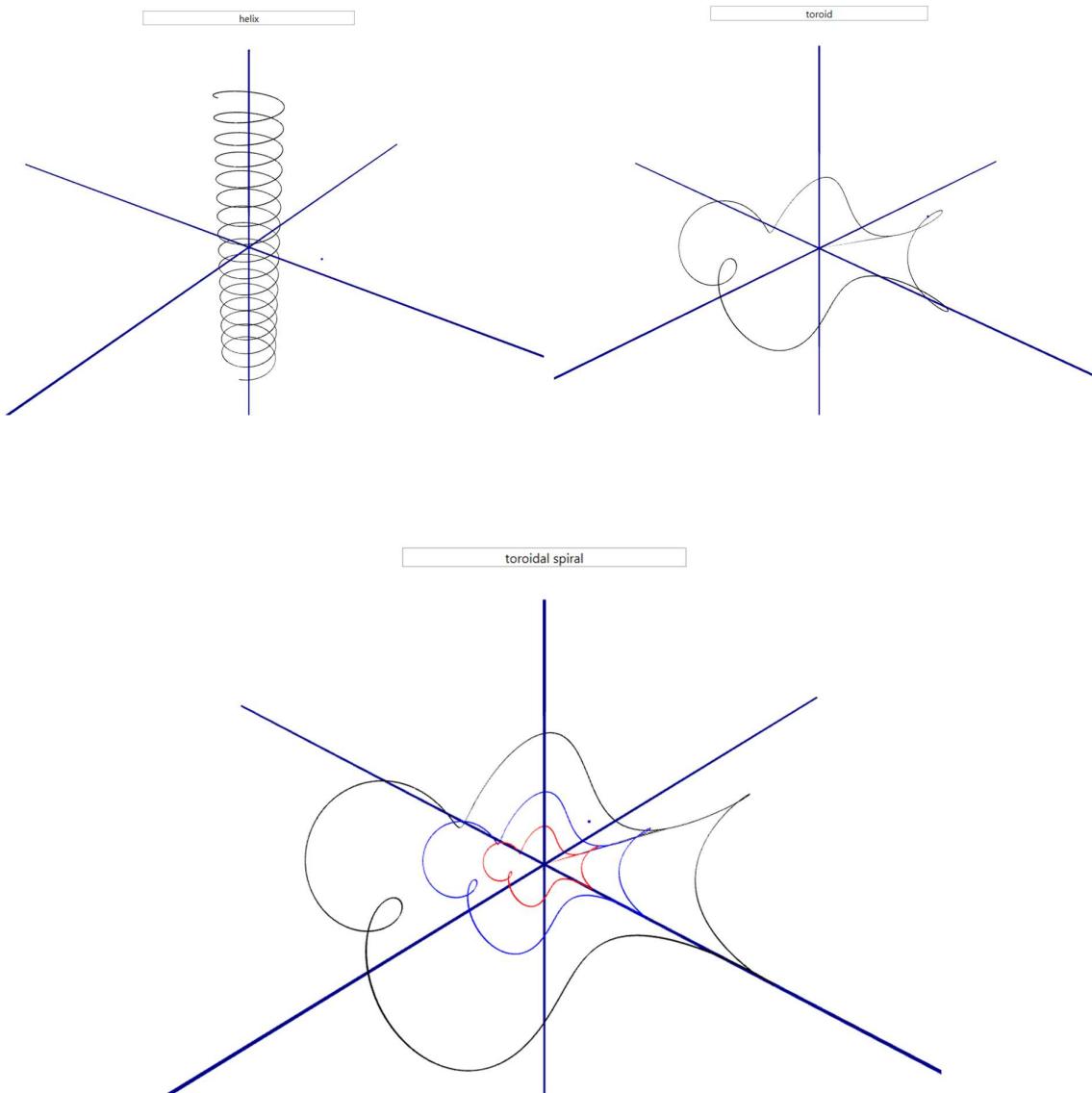
Generated content of file "example3_wpf_curve_helix.txt":

```

PARAMETRIC_CURVE_CARTESIAN_3D
helix
t1: -50
t2: 50
NumPoints: 1000
-50 19.2993 5.2475 -100
-49.8999 18.6783 7.14987 -99.7998
-49.7998 17.8703 8.98066 -99.5996
-49.6997 16.8834 10.7215 -99.3994

```

```
-49.5996 15.7274 12.3551 -99.1992
...
49.4995 14.414 -13.8649 98.999
49.5996 15.7274 -12.3551 99.1992
49.6997 16.8834 -10.7215 99.3994
49.7998 17.8703 -8.98066 99.5996
49.8999 18.6783 -7.14987 99.7998
50 19.2993 -5.2475 100
```



What if we have parametric curve given by a list of points?

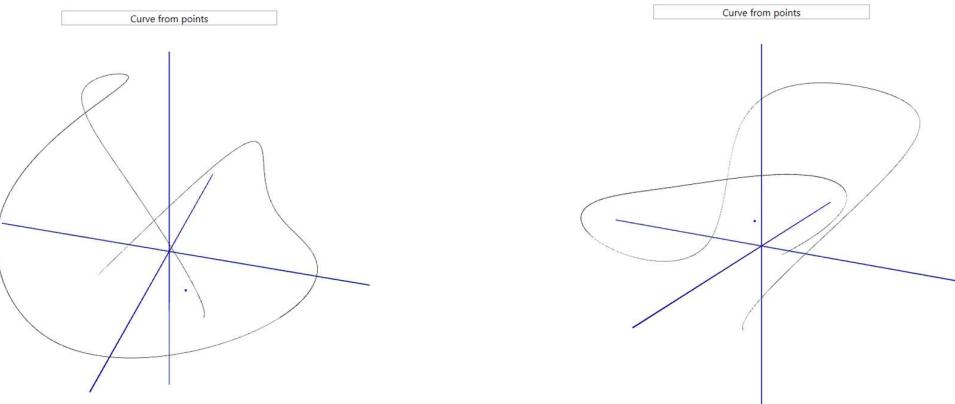
```

// First case - we already have points in Matrix
Matrix<Real> curve_points1{ 10, 3,
{
    {0.0, 50.0, -100.0,
     -100.0,-100.0, 50.0,
     -150.0,-180.0, 150.0,
     -80.0, -80.0, 200.0,
     130.0,-150.0, 100.0,
     150.0,-100.0, -50.0,
     100.0, 180.0, 90.0,
     50.0, 140.0, 100.0,
     -70.0, 100.5, 120.0,
     20.0, -100.5, -50.0}};

// we can easily create spline parametric curve
SplineInterpParametricCurve<3> curve(0.0, 1.0, curve_points1);

Visualizer::VisualizeParamCurve3D(curve, "Curve from points", 0.0, 1.0, 1000,
"example3_wpf_curve_spline.txt");

```



Visualizing Lorentz system solution as parametric curve in 3D.

```

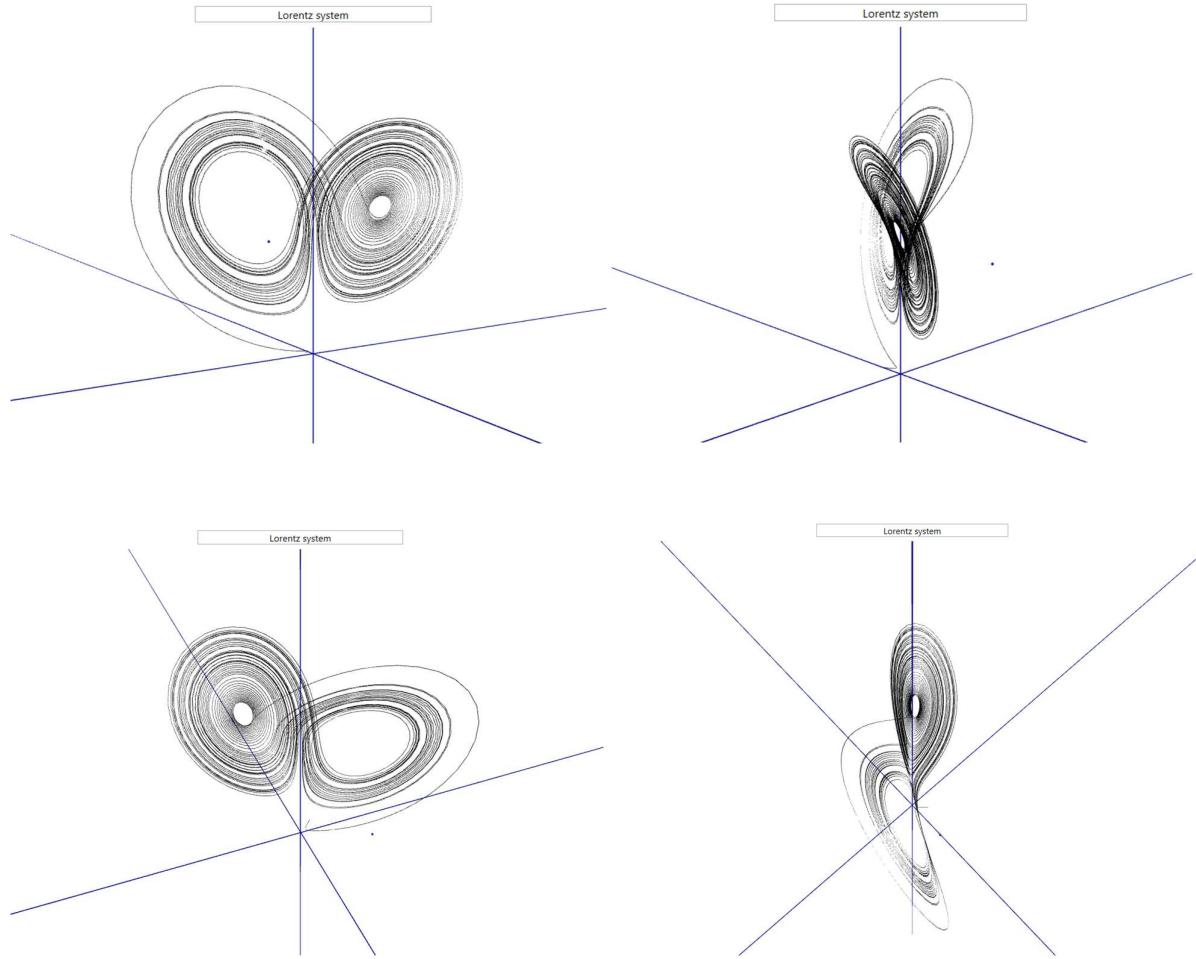
// Lorentz system as 3D parametric curve
ODESystem lorentz_system(3, [](Real t, const Vector<Real>& x, Vector<Real>& dxdt)
{
    const Real sigma = 10.0;
    const Real rho = 28.0;
    const Real beta = 8.0 / 3.0;
    dxdt[0] = sigma * (x[1] - x[0]);
    dxdt[1] = x[0] * (rho - x[2]) - x[1];
    dxdt[2] = x[0] * x[1] - beta * x[2];
};

Vector<Real> ystart({ -2.0, 3.0, 1.0 });
ODESystemSolver<RK5_CashKarp_Stepper> solver(lorentz_system);

ODESystemSolution sol = solver.integrate(ystart, 0.0, 50.0, 0.001, 1e-08, 0.01);

SplineInterpParametricCurve<3> solCurve1 = sol.getSolutionAsParametricCurve3D(0, 1, 2);
Visualizer::VisualizeODESysSolAsParamCurve3(sol, 0, 1, 2, "Lorentz system",
"example3_wpf_lorentz_system1.txt");

```



Adding more initial conditions.

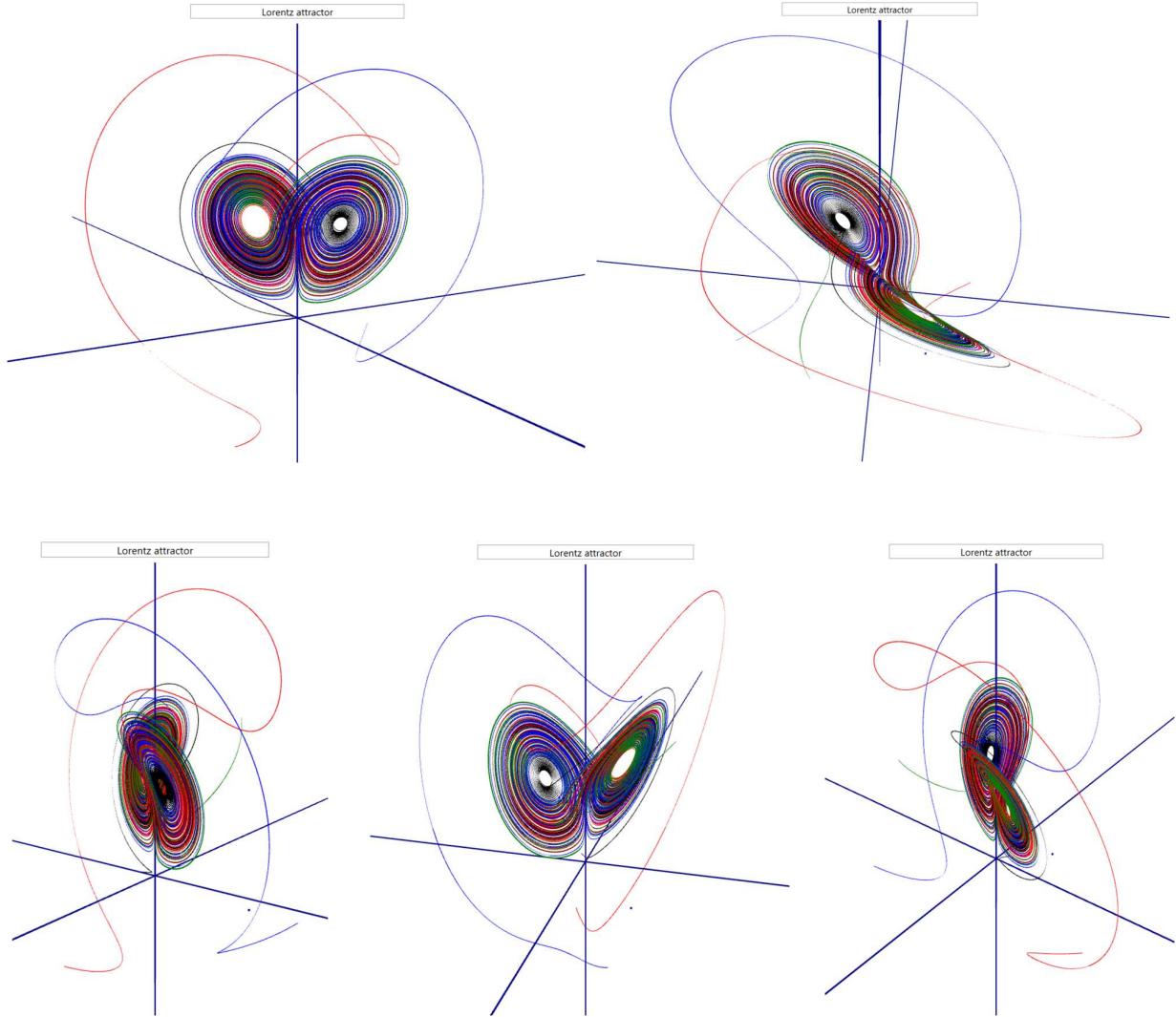
```

Vector<Real> ystart1({5.0,-15.0,-10.0}), ystart2({-10.0,25.0,-3.0}), ystart3({15.0,-10.0,5.0});

sol = solver.integrate(ystart1, 0.0, 50.0, 0.001, 1e-10, 0.001);
SplineInterpParametricCurve<3> solCurve2 = sol.getSolutionAsParametricCurve3D(0, 1, 2);
sol = solver.integrate(ystart2, 0.0, 50.0, 0.001, 1e-10, 0.001);
SplineInterpParametricCurve<3> solCurve3 = sol.getSolutionAsParametricCurve3D(0, 1, 2);
sol = solver.integrate(ystart3, 0.0, 50.0, 0.001, 1e-10, 0.001);
SplineInterpParametricCurve<3> solCurve4 = sol.getSolutionAsParametricCurve3D(0, 1, 2);

// visualize together
Visualizer::VisualizeMultiParamCurve3D({ &solCurve1, &solCurve2 }, "Lorentz system",
                                         0.0, 50.0, 10000, "example3_wpf_lorentz_system_multi.txt");

```



Visualizer for parametric curves also has animation capability, where each curve is visualized by a moving little sphere, following curve progressss.

Visualizing surfaces

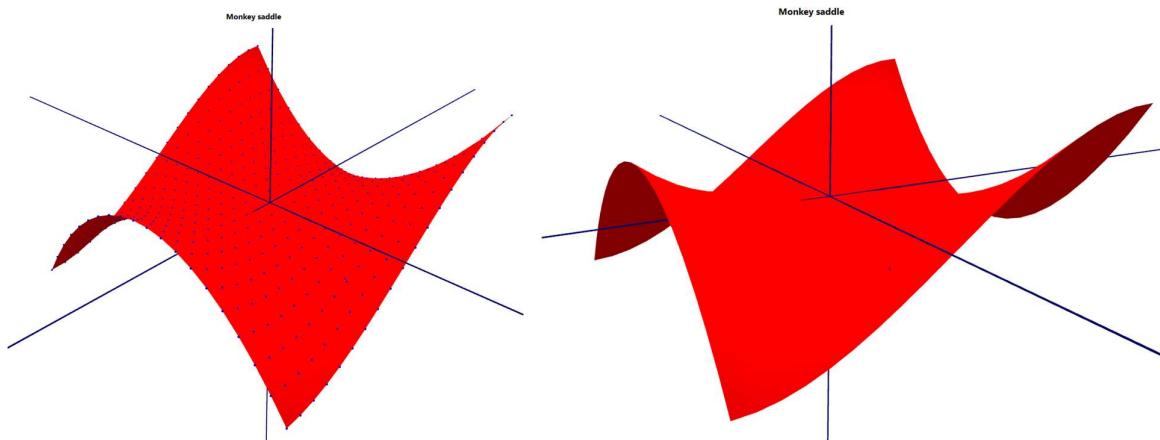
```
// Monkey saddle surface
ScalarFunction<2> testFunc1{ [] (const VectorN<Real, 2>& x)
{
    return 3 * x[0] / 5 * (x[0] * x[0] / 25 - 3 * x[1] * x[1] / 25);
};

Visualizer::VisualizeScalarFunc2DCartesian(testFunc1, "Monkey saddle",
-10.0, 10.0, 20, -10.0, 10.0, 20,
"example3_wpf_surface1.txt");
```

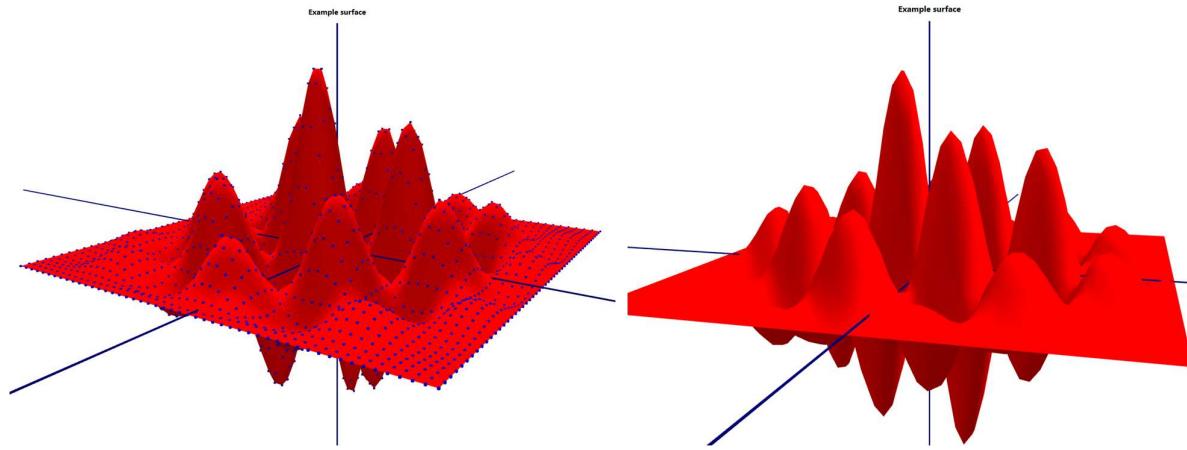
Generated content in file:

```
SCALAR_FUNCTION_CARTESIAN_2D
Monkey saddle
x1: -10
x2: 10
NumPointsX: 20
y1: -10
y2: 10
NumPointsY: 20
-10 -10 48
-10 -8.94737 33.6399
-10 -7.89474 20.8753
-10 -6.84211 9.70637
-10 -5.78947 0.132964
-10 -4.73684 -7.84488
-10 -3.68421 -14.2271
...
10 2.63158 19.0139
10 3.68421 14.2271
10 4.73684 7.84488
10 5.78947 -0.132964
10 6.84211 -9.70637
10 7.89474 -20.8753
10 8.94737 -33.6399
10 10 -48
```

Visualizations (with and without markings for surface points).



Second example.



Visualizing 2D & 3D vector fields

Visualizing vector field in 2 dimensions.

```
VectorFunction<2> rotational_field{ [] (const VectorN<Real, 2>& x)
{
    Real norm = x.NormL2();
    return VectorN<Real, 2>{-x[1] / norm, x[0] / norm};
};

Visualizer::VisualizeVectorField2DCartesian(rotational_field, "rotational_field",
                                            -10.0, 10.0, 20, -10.0, 10.0, 20,
                                            "example3_wpf_vector_field_2d.txt");
```

Generated content in file.

```
VECTOR_FIELD_2D_CARTESIAN
rotational_field
-10 -10 0.707107 -0.707107
-10 -8.94737 0.666795 -0.745241
-10 -7.89474 0.619644 -0.784883
-10 -6.84211 0.564684 -0.825307
-10 -5.78947 0.501036 -0.865426
-10 -4.73684 0.428086 -0.903738
-10 -3.68421 0.345705 -0.938343
...
10 4.73684 -0.428086 0.903738
10 5.78947 -0.501036 0.865426
10 6.84211 -0.564684 0.825307
10 7.89474 -0.619644 0.784883
```

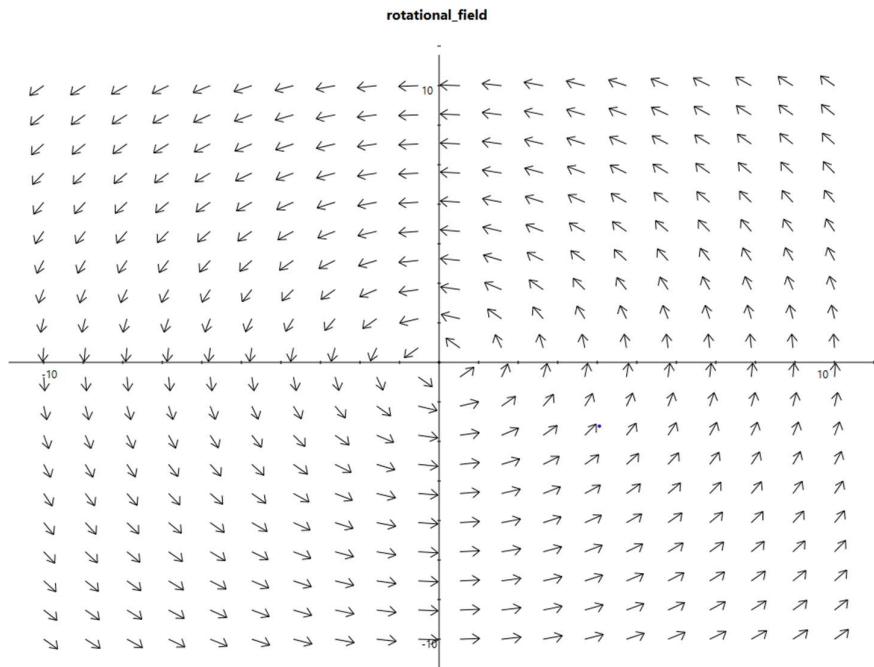
```

10 8.94737 -0.666795 0.745241
10 10 -0.707107 0.707107

```

Absence of x_1 , x_2 , NumPoints and similar parameters is due to the fact that visualizer component performs automatic analysis of input domain, so even though our serializer will save values in neat pattern, that is not a requirement.

Visualization.



Visualizing vector fields in 3 dimensions

```

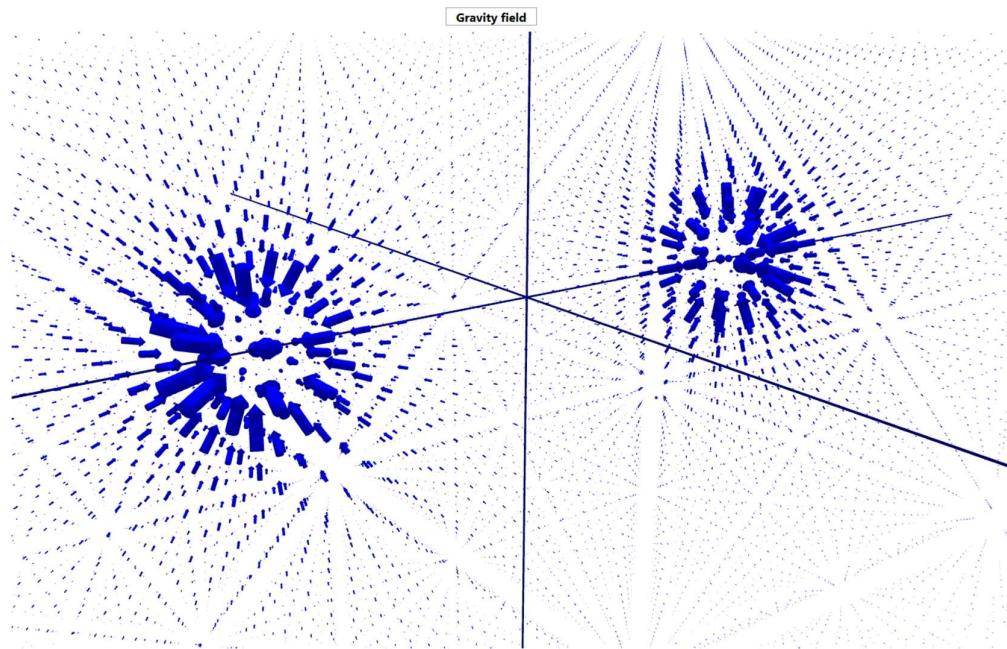
// defining force field of two masses as VectorFunction
VectorFunction<3> gravity_force_field{ [](const VectorN<Real, 3>& x)
{
    const VectorN<Real, 3> x1{ 100, 0, 0}, x2{ -100, 0, 0};
    const Real m1 = 100.0, m2 = 100.0;
    const Real G = 10;
    return -G * m1 * (x - x1) / std::pow((x - x1).NormL2(), 3) -
        G * m2 * (x - x2) / std::pow((x - x2).NormL2(), 3);
} };

Visualizer::VisualizeVectorField3DCartesian(gravity_force_field, "Gravity field",
    -200, 200, 30, -200, 200, 30, -200, 200, 30,
    "example3_wpf_vector_field_3d.txt");

```

Generated file content.

```
VECTOR_FIELD_3D_CARTESIAN
Gravity field
-200 -200 -200 0.00798374 0.0102608 0.0102608
-200 -200 -186.207 0.00854805 0.0111102 0.010344
-200 -200 -172.414 0.00914172 0.0120174 0.0103598
-200 -200 -158.621 0.00976156 0.0129785 0.0102933
-200 -200 -144.828 0.0104026 0.0139866 0.0101282
-200 -200 -131.034 0.0110579 0.015031 0.00984791
...
200 200 144.828 -0.0104026 -0.0139866 -0.0101282
200 200 158.621 -0.00976156 -0.0129785 -0.0102933
200 200 172.414 -0.00914172 -0.0120174 -0.0103598
200 200 186.207 -0.00854805 -0.0111102 -0.010344
200 200 200 -0.00798374 -0.0102608 -0.0102608
```



Visualizing particle simulations

Still a work in progress!

Used mostly for Collision simulator in Chapter 4, and N-body gravity simulation in Chapter 9

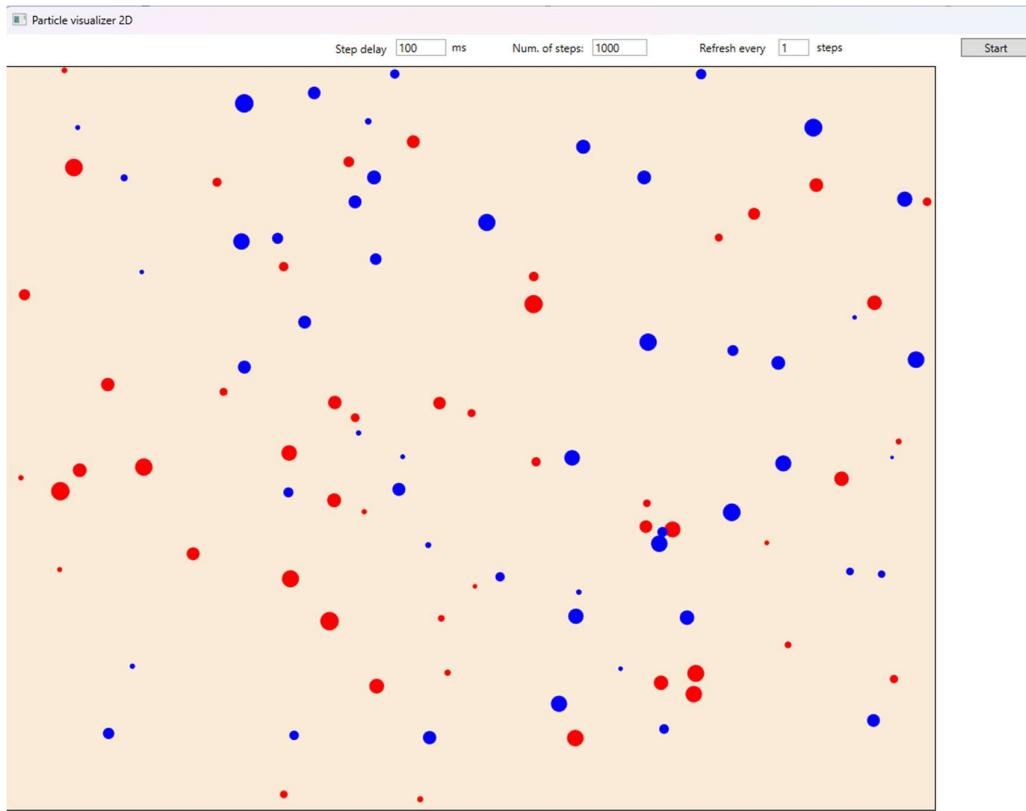
Enables visualization of N particles/bodies trajectories.

Particle simulation in 2D

Generated file with 100 balls (50 red, 50 blue), with random radii (in interval [3, 10]), and random positions within container 1000 x 1000

File format:

```
PARTICLE_SIMULATION_DATA_2D
NumBalls: 100
Ball_1 Red 6.50868
Ball_2 Red 9.1677
Ball_3 Red 6.10828
Ball_4 Red 3.32719
Ball_5 Red 5.02304
Ball_6 Red 7.30436
...
Ball_95 Blue 5.1793
Ball_96 Blue 7.86956
Ball_97 Blue 4.18073
Ball_98 Blue 9.2595
Ball_99 Blue 2.72341
Ball_100 Blue 7.5783
...
NumSteps: 1000
Step 0 0.1
0 804.722 158.636
1 742.083 652.353
2 20.9098 245.59
3 446.054 787.569
...
97 517.628 167.955
98 78.0881 65.9395
99 396.442 119.555
Step 1 0.1
0 804.52 159.486
1 745.673 649.094
2 19.5543 241.504
3 441.1 783.76
...
96 373.656 241.988
97 731.294 513.615
98 491.409 292.996
99 872.334 719.965
```



Particle simulation in 3D

Same as in previous example, but in 3D.

Generated file with trajectory data for 100 balls.

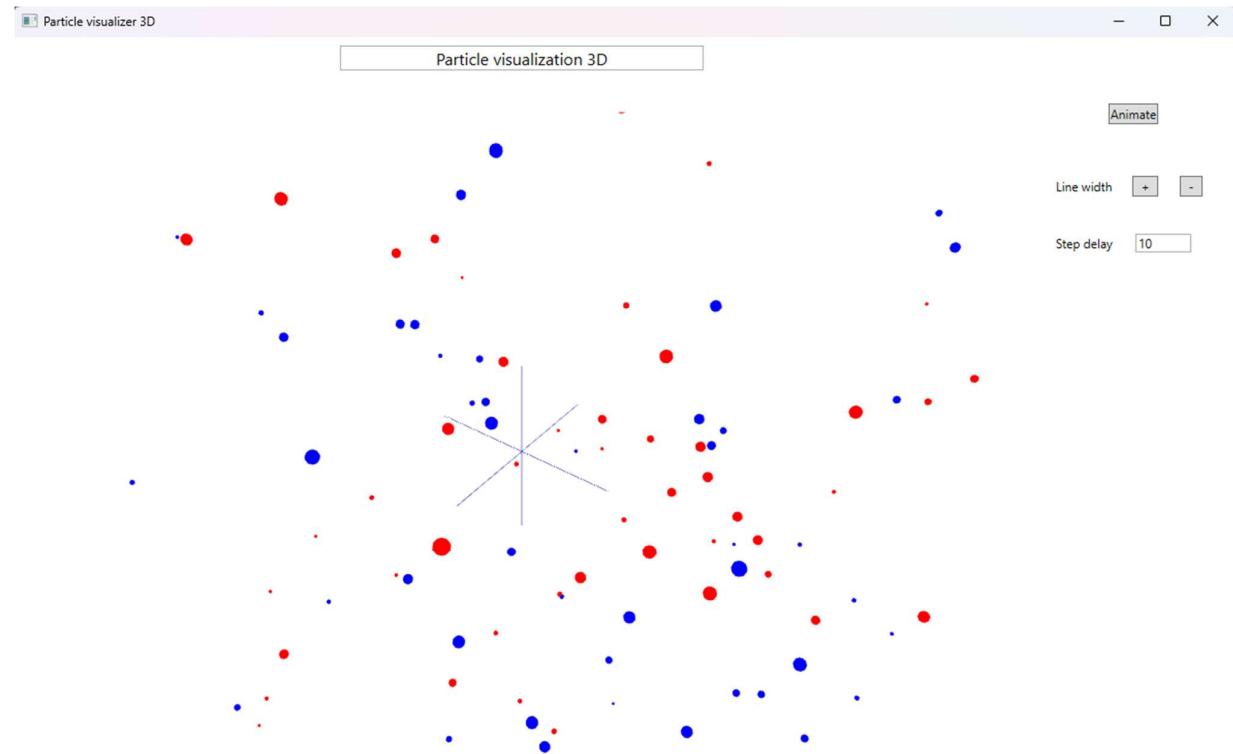
```
PARTICLE_SIMULATION_DATA_3D
NumBalls: 100
Ball_1 Red 8.2318
Ball_2 Red 8.1955
Ball_3 Red 3.45126
Ball_4 Red 7.48618
Ball_5 Red 3.66358
...
Ball_95 Blue 9.62492
Ball_96 Blue 8.90473
Ball_97 Blue 5.57198
Ball_98 Blue 9.37226
Ball_99 Blue 9.64663
Ball_100 Blue 6.69845
...
NumSteps: 100
Step 0 0.1
0 972.958 635.321 816.846
1 249.184 519.539 311.393
```

```

2 609.546 167.804 180.063
3 330.283 60.1874 701.593
4 115.636 292.918 219.628
5 181.193 119.617 137.269
...
96 269.386 601.865 499.579
97 567.563 741.41 153.786
98 576.764 161.905 137.72
99 158.822 830.989 838.669
Step 1 0.1
0 977.84 640.037 814.508
1 254.142 518.377 314.322
2 608.054 163.256 180.617
3 334.326 56.7461 701.798
...
95 46.8158 184.978 186.921
96 753.494 808.642 800.327
97 276.137 806.593 81.3732
98 802.489 195.024 298.528
99 74.7379 503.788 695.406

```

Visualization



3. Basic algorithms

Putting some algorithmic meat on our objects.

SOLVING SYSTEMS OF LINEAR EQUATIONS

General introduction

$$\begin{aligned} a_{00}x_0 + a_{01}x_1 + a_{02}x_2 + \cdots + a_{0,N-1}x_{N-1} &= b_0 \\ a_{10}x_0 + a_{11}x_1 + a_{12}x_2 + \cdots + a_{1,N-1}x_{N-1} &= b_1 \\ a_{20}x_0 + a_{21}x_1 + a_{22}x_2 + \cdots + a_{2,N-1}x_{N-1} &= b_2 \\ &\dots &&\dots \\ a_{M-1,0}x_0 + a_{M-1,1}x_1 + \cdots + a_{M-1,N-1}x_{N-1} &= b_{M-1} \end{aligned}$$

TODO - Little bit of algebra – singular matrices, rank, kernel, null space

Gauss-Jordan

Starting with the basic Gauss-Jordan elimination algorithm ... THAT SHOULD NEVER BE USED!

Gauss-Jordan with pivoting

This is what you should (at minimum) be using.

```
//////////////////////////////////////////////////////////////// GAUSS-JORDAN SOLVER //////////////////////////////
template<class Type>
class GaussJordanSolver
{
public:
    // solving with Matrix RHS (ie. solving simultaneously for multiple RHS)
    static bool Solve(Matrix<Type>& a, Matrix<Type>& b){ ... }

    // solving for a given RHS vector
    static bool Solve(Matrix<Type>& a, Vector<Type>& b){ ... }

    // solving for a given RHS vector, but with return value
    // (in case of singular matrix 'a', exception is thrown)
    static Vector<Type> SolveConst(Matrix<Type>& a, const Vector<Type>& b){ ... }
};
```

LU decomposition

Solving iteratively – Jacoby, Gauss-Seidel, SOR

Example usage – solving systems of linear equations

https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/Chapter_02_basic_algorithms/demo_lin_alg_sys_solvers.cpp

```
// initialize a 4x4 matrix, defining the system of linear equations
Matrix<Real> mat(4, 4, { -2, 4, 3, 5,
                           3, 8, -7, -2,
                           1, -3, 7, 4,
                           5, -4, 9, 1 });
Matrix<Real> matcopy(mat);
std::cout << "Initial matrix:\n"; mat.Print(std::cout, 10, 3);

// right side vector
Vector<Real> rhs({ 3, -2, 1, 5 }), rhscopy(rhs);
std::cout << "\nRight side: "; rhs.Print(std::cout, 10, 3);

// solution is returned in rhs vector
GaussJordanSolver<Real>::Solve(mat, rhs);

Vector<Real> sol2 = GaussJordanSolver<Real>::SolveConst(matcopy, rhscopy);

std::cout << "\nSolution: " << rhs << std::endl;
std::cout << "mat * sol = "; (matcopy * rhs).Print(std::cout, 10, 3);
```

Program output

```
Initial matrix:
Rows: 4 Cols: 4
[      -2,          4,          3,          5 ]
[      3,          8,         -7,         -2 ]
[      1,         -3,          7,          4 ]
[      5,         -4,          9,          1 ]
Right side: [      3,         -2,          1,          5]
Solution: [ -0.8427672956,    1.150943396,   1.72327044, -1.691823899]
mat * sol = [     1.03,      -1.01,      -1.42,       1.9]
```

NUMERICAL DERIVATION

Most of the code here is based on Boost.Math toolkit, and its differentiation routines.

Mathematics of derivation approximation

Simple, right?

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

Taylor expansion and all that jazz.

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \frac{1}{6}h^3 f'''(x) + \dots$$

Central difference is better, because it is a *second order* method

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

And it comes down to (mostly) properly handling value of 'h', depending on the order

Calculating second and third derivations

TODO

Derivation routines

Default step-sizes for routines of different order, defined in terms of machine Real type epsilon

```
static inline const Real NDer1_h = 2 * std::sqrt(Constants::Epsilon);
static inline const Real NDer2_h = std::pow(3 * Constants::Epsilon, 1.0 / 3.0);
static inline const Real NDer4_h = std::pow(11.25 * Constants::Epsilon, 1.0 / 5.0);
static inline const Real NDer6_h = std::pow(Constants::Epsilon / 168.0, 1.0 / 7.0);
static inline const Real NDer8_h = std::pow(551.25 * Constants::Epsilon, 1.0 / 9.0);
```

As an example, here is first order derivation of a RealFunction

```
static Real NDer1(const IRealFunction& f, Real x, Real h, Real* error = nullptr)
{
    Real yh = f(x + h);
    Real y0 = f(x);
    Real diff = yh - y0;
    if (error)
    {
        Real ym = f(x - h);
        Real ypph = std::abs(yh - 2 * y0 + ym) / h;

        *error = ypph / 2 + (std::abs(yh) + std::abs(y0)) * Constants::Eps / h;
    }
    return diff / h;
}
```

Second order method, using central difference.

```
static Real NDer2(const IRealFunction& f, Real x, Real h, Real* error = nullptr)
{
    Real yh = f(x + h);
    Real ymh = f(x - h);
    Real diff = yh - ymh;
    if (error)
    {
        Real y2h = f(x + 2 * h);
        Real ym2h = f(x - 2 * h);
        *error = Constants::Eps * (std::abs(yh) + std::abs(ymh)) / (2 * h) +
                 std::abs((y2h - ym2h) / 2 - diff) / (6 * h);
    }
    return diff / (2 * h);
}
```

Calculating fourth order derivation requires four function evaluations.

```
static Real NDer4(const IRealFunction& f, Real x, Real h, Real* error = nullptr)
{
    Real yh = f(x + h);
    Real ymh = f(x - h);
    Real y2h = f(x + 2 * h);
    Real ym2h = f(x - 2 * h);

    Real y2 = ym2h - y2h;
    Real y1 = yh - ymh;

    if (error)
    {
        // ...
        Real y3h = f(x + 3 * h);
        Real ym3h = f(x - 3 * h);

        // Error from fifth derivative:
        *error = std::abs(y3h - ym3h) / 2 + 2 * (ym2h - y2h) + 5 * (yh - ymh) / 2) / (30 * h);
        // Error from function evaluation:
        *error += Constants::Epsilon * (std::abs(y2h) + std::abs(ym2h) +
                                         8 * (std::abs(ymh) + std::abs(yh))) / (12 * h);
    }
    return (y2 + 8 * y1) / (12 * h);
}
```

Fourth order (partial) derivation of ScalarFunction (we have to specify by which index we are deriving)

```
template <int N>
static Real NDer4Partial(const IScalarFunction<N>& f, int deriv_index, const VectorN<Real, N>& point,
                        Real h, Real* error = nullptr)
{
    Real orig_x = point[deriv_index];

    VectorN<Real, N> x{ point };
    x[deriv_index] = orig_x + h;
    Real yh = f(x);

    x[deriv_index] = orig_x - h;
    Real ymh = f(x);

    x[deriv_index] = orig_x + 2 * h;
    Real y2h = f(x);

    x[deriv_index] = orig_x - 2 * h;
    Real ym2h = f(x);

    Real y2 = ym2h - y2h;
    Real y1 = yh - ymh;

    if (error)
    {
        x[deriv_index] = orig_x + 3 * h;
        Real y3h = f(x);

        x[deriv_index] = orig_x - 3 * h;
        Real ym3h = f(x);

        *error = std::abs((y3h - ym3h) / 2 + 2 * (ym2h - y2h) + 5 * (yh - ymh) / 2) / (30 * h);
        *error += Constants::Epsilon * (std::abs(y2h) + std::abs(ym2h) +
                                         8 * (std::abs(ymh) + std::abs(yh))) / (12 * h);
    }
    return (y2 + 8 * y1) / (12 * h);
}
```

And a similar example for deriving VectorFunction (of second order, for simplicity), where we have to specify both function index, and index of variable we want to derive by).

```

template <int N>
static Real NDer2Partial(const IVectorFunction<N>& f, int func_index, int deriv_index,
                       const VectorN<Real, N>& point, Real h, Real* error = nullptr)
{
    Real orig_x = point[deriv_index];

    VectorN<Real, N> x{ point };
    x[deriv_index] = orig_x + h;
    Real yh = f(x)[func_index];

    x[deriv_index] = orig_x - h;
    Real ymh = f(x)[func_index];

    Real diff = yh - ymh;

    if (error)
    {
        x[deriv_index] = orig_x + 2 * h;
        Real y2h = f(x)[func_index];

        x[deriv_index] = orig_x - 2 * h;
        Real ym2h = f(x)[func_index];

        *error = Constants::Epsilon * (std::abs(yh) + std::abs(ymh)) / (2 * h) +
                 std::abs((y2h - ym2h) / 2 - diff) / (6 * h);
    }
}

return diff / (2 * h);
}

```

RealFunction derivation routines

Given are definitions only for first order, but, as with all other types, all presented functions are available up to 8th order.

```

static Real NDer1(const IRealFunction& f, Real x, Real h, Real* error = nullptr){ ... }
static Real NDer1(const IRealFunction& f, Real x, Real* error){ ... }
static Real NDer1(const IRealFunction& f, Real x){ ... }

static Real NDer1Left(const IRealFunction& f, Real x, Real* error = nullptr){ ... }
static Real NDer1Right(const IRealFunction& f, Real x, Real* error = nullptr){ ... }
static Real NDer1Left(const IRealFunction& f, Real x, Real h, Real* error = nullptr){ ... }
static Real NDer1Right(const IRealFunction& f, Real x, Real h, Real* error = nullptr){ ... }

```

For RealFunction we also have second and third derivations

```

static Real NSecDer1(const IRealFunction& f, Real x, Real h, Real* error = nullptr){ ... }
static Real NSecDer1(const IRealFunction& f, Real x, Real* error = nullptr){ ... }

static Real NThirdDer1(const IRealFunction& f, Real x, Real h, Real* error = nullptr){ ... }
static Real NThirdDer1(const IRealFunction& f, Real x, Real* error = nullptr){ ... }

```

ScalarFunction derivation routines

```
template <int N>
static Real NDeriPartial(const IScalarFunction<N>& f, int deriv_index, const VectorN<Real, N>& point,
                           Real h, Real* error = nullptr) { ... }

template <int N>
static Real NDeriPartial(const IScalarFunction<N>& f, int deriv_index, const VectorN<Real, N>& point,
                           Real* error = nullptr) { ... }

template <int N>
static VectorN<Real, N> NDeriPartialByAll(const IScalarFunction<N>& f, const VectorN<Real, N>& point,
                                              Real h, VectorN<Real, N>* error = nullptr) { ... }

template <int N>
static VectorN<Real, N> NDeriPartialByAll(const IScalarFunction<N>& f, const VectorN<Real, N>& point,
                                              VectorN<Real, N>* error = nullptr) { ... }
```

We can also calculate second partial derivations for ScalarFunction

```
template <int N>
static Real NSecDeriPartial(const IScalarFunction<N>& f, int der_ind1, int der_ind2,
                           const VectorN<Real, N>& point, Real h, Real* error = nullptr) { ... }

template <int N>
static Real NSecDeriPartial(const IScalarFunction<N>& f, int der_ind1, int der_ind2,
                           const VectorN<Real, N>& point, Real* error = nullptr) { ... }
```

VectorFunction derivation routines

```
template <int N>
static Real NDeriPartial(const IVectorFunction<N>& f, int func_index, int deriv_index,
                        const VectorN<Real, N>& point, Real h, Real* error = nullptr) { ... }

template <int N>
static Real NDeriPartial(const IVectorFunction<N>& f, int func_index, int deriv_index,
                        const VectorN<Real, N>& point, Real* error = nullptr) { ... }

template <int N>
static VectorN<Real, N> NDeriPartialByAll(const IVectorFunction<N>& f, int func_index,
                                             const VectorN<Real, N>& point, Real h, VectorN<Real, N>* error = nullptr)

template <int N>
static VectorN<Real, N> NDeriPartialByAll(const IVectorFunction<N>& f, int func_index,
                                             const VectorN<Real, N>& point, VectorN<Real, N>* error = nullptr)

template <int N>
static MatrixNM<Real, N, N> NDeriPartialAllByAll(const IVectorFunction<N>& f, const VectorN<Real, N>& point,
                                                 Real h, MatrixNM<Real, N, N>* error = nullptr) { ... }

template <int N>
static MatrixNM<Real, N, N> NDeriPartialAllByAll(const IVectorFunction<N>& f, const VectorN<Real, N>& point,
                                                 MatrixNM<Real, N, N>* error = nullptr) { ... }
```

ParametricCurve derivation routines

```
template <int N>
static VectorN<Real, N> NDeri1(const IParametricCurve<N>& f, Real t, Real h, Real* error = nullptr) { ... }

template <int N>
static VectorN<Real, N> NDeri1(const IParametricCurve<N>& f, Real t, Real* error = nullptr) { ... }
```

Second and third derivations are also available for ParametricCurve

```
template <int N>
static VectorN<Real, N> NSecDer1(const IParametricCurve<N>& f, Real x, Real h, Real* error = nullptr) { ... }
template <int N>
static VectorN<Real, N> NSecDer1(const IParametricCurve<N>& f, Real x, Real h, Real* error = nullptr) { ... }

template <int N>
static VectorN<Real, N> NThirdDer1(const IParametricCurve<N>& f, Real x, Real h, Real* error = nullptr) { ... }
template <int N>
static VectorN<Real, N> NThirdDer1(const IParametricCurve<N>& f, Real x, Real h, Real* error = nullptr) { ... }
```

Examples of usage - derivation

https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/Chapter_02_basic_algorithms/demo_derivation.cpp

RealFunction derivation examples

```
RealFunction      f1{ [](Real x) { return (Real)(sin(x) * (1.0 + 0.5 * x * x)); } };

// numerical derivation of real function (available orders - 1, 2, 4, 6, 8)
double der_f1 = Derivation::NDer1(f1, 0.5);
double der_f2 = Derivation::NDer2(f1, 0.5, 1e-6);    // setting explicit step size
Real err;
double der_f6 = Derivation::NDer6(f1, 0.5, &err);   // if we need error estimate
double der_f8 = Derivation::NDer8(f1, 0.5);

// we can use default Derive routine (set to NDer4)
double der_f4 = Derivation::Derive(f1, 0.5);
// available also with error estimate
double der_f41 = Derivation::DeriveErr(f1, 0.5, &err);

// second and third derivatives
double sec_der_f1  = Derivation::NSecDer2(f1, 0.5);
double third_der_f1 = Derivation::NThirdDer2(f1, 0.5);
```

Scalar and vector functions

```
ScalarFunction<3>  f2Scal([](const VectorN<Real, 3>& x) { return (Real)(1.0 / pow(x.NormL2(), 2)); });
VectorFunction<3>  f3Vec([](const VectorN<Real, 3>& x) { return VectorN<Real, 3>{0, x[0] * x[1], 0}; });

VectorN<Real, 3> der_point{ 1.0, 1.0, 1.0 };

double      der_f2Scal     = Derivation::NDer1Partial(f2Scal, 1, der_point);
VectorN<Real, 3> der_f2Scal_all = Derivation::NDer1PartialByAll(f2Scal, der_point);

double      der_f3Vec      = Derivation::NDer1Partial(f3Vec, 1, 1, der_point);
VectorN<Real, 3> der_f3Vec_by1  = Derivation::NDer2PartialByAll(f3Vec, 1, der_point);
MatrixNM<Real, 3, 3> der_f3Vec_by_all = Derivation::NDer4PartialAllByAll(f3Vec, der_point);
```

Parametric curve

```
ParametricCurve<3> f4Curve([](Real x) { return VectorN<Real, 3>{x, 2 * x, 3 * x}; });

VectorN<Real, 3> der_f4Curve = Derivation::NDer1(f4Curve, 1.0);
VectorN<Real, 3> sec_f4Curve = Derivation::NSecDer1(f4Curve, 1.0);
VectorN<Real, 3> third_f4Curve = Derivation::NThirdDer1(f4Curve, 1.0);
```

Automatic differentiation

Short overview of basic AD implementation

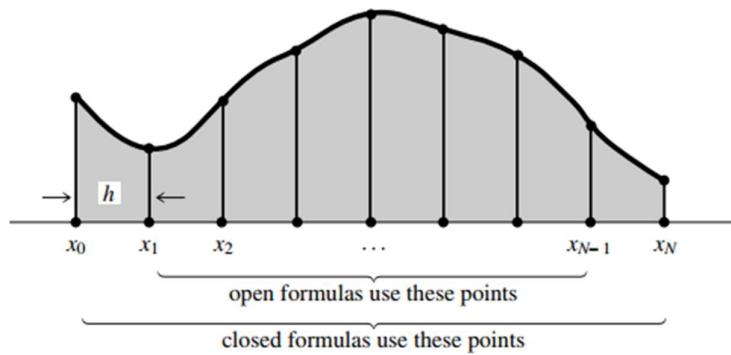
NUMERICAL INTEGRATION

We want so solve this

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

For a given function f , and limits a and b .

Open vs closed formulas.



Basic trapezoidal rule for approximation in single interval.

$$\int_{x_0}^{x_1} f(x)dx = h \left[\frac{1}{2}f_0 + \frac{1}{2}f_1 \right] + O(h^3 f'')$$

Simpson's rule

$$\int_{x_0}^{x_2} f(x)dx = h \left[\frac{1}{3}f_0 + \frac{4}{3}f_1 + \frac{1}{3}f_2 \right] + O(h^5 f^{(4)})$$

Extended trapezoidal rule.

$$\begin{aligned} \int_{x_0}^{x_{N-1}} f(x)dx = h & \left[\frac{1}{2}f_0 + f_1 + f_2 + \right. \\ & \left. \dots + f_{N-2} + \frac{1}{2}f_{N-1} \right] + O\left(\frac{(b-a)^3 f''}{N^2}\right) \end{aligned}$$

Trapezoidal integrator

Basic interface, because all integrators are “refinement machines”, calculating with more and more interior points, until required accuracy is achieved.

<https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/mml/core/Integration.h>

```
enum IntegrationMethod { TRAP, SIMPSON, ROMBERG, GAUSS10 };

class IQuadrature {
public:
    int _currStep;
    virtual Real next() = 0;
};
```

Implementation of trapezoidal refinement step

```
class TrapIntegrator : IQuadrature
{
public:
    Real _a, _b, _currSum;
    const IRealFunction& _func;

    TrapIntegrator(const IRealFunction& func, Real aa, Real bb) :
        _func(func), _a(aa), _b(bb), _currSum(0.0) { _currStep = 0; }

    // ...
    Real next() {
        Real x, sum, del;
        int subDivNum, j;

        _currStep++;
        if (_currStep == 1) {
            return (_currSum = 0.5 * (_b - _a) * (_func(_a) + _func(_b)));
        }
        else {
            for (subDivNum = 1, j = 1; j < _currStep - 1; j++)
                subDivNum *= 2;

            del = (_b - _a) / subDivNum;
            x = _a + 0.5 * del;

            for (sum = 0.0, j = 0; j < subDivNum; j++, x += del)
                sum += _func(x);

            _currSum = 0.5 * (_currSum + (_b - _a) * sum / subDivNum);
        }
        return _currSum;
    }
};
```

Implementation of trapezoidal integration function

```
static Real IntegrateTrap(const IRealFunction& func, Real a, Real b,
                           int* doneSteps, Real* achievedPrec,
                           const Real eps = Defaults::TrapezoidIntegrationEPS)
{
    Real currSum, oldSum = 0.0;

    TrapIntegrator t(func, a, b);

    for (int j = 0; j < Defaults::TrapezoidIntegrationMaxSteps; j++)
    {
        currSum = t.next();

        if (j > 5) {
            if (std::abs(currSum - oldSum) < eps * std::abs(oldSum) ||
                (currSum == 0.0 && oldSum == 0.0))
            {
                if (doneSteps != nullptr) *doneSteps = j;
                if (achievedPrec != nullptr) *achievedPrec = std::abs(currSum - oldSum);
            }
            return currSum;
        }

        oldSum = currSum;
    }

    if (doneSteps != nullptr) *doneSteps = Defaults::TrapezoidIntegrationMaxSteps;
    if (achievedPrec != nullptr) *achievedPrec = std::abs(currSum - oldSum);

    return currSum;
}
```

Gauss-Legendre integration

```
static Real IntegrateGauss10(const IRealFunction& func, const Real a, const Real b)
{
    // Returns the integral of the function func between a and b, by ten-point GaussLegendre integration:
    // the function is evaluated exactly ten times at interior points in the range of integration.
    static const Real x[] = { 0.1488743389816312, 0.4333953941292472,
                             0.6794095682990244, 0.8650633666889845, 0.9739065285171717 };
    static const Real w[] = { 0.2955242247147529, 0.2692667193099963,
                             0.2190863625159821, 0.1494513491505806, 0.0666713443086881 };

    Real xm = 0.5 * (b + a);
    Real xr = 0.5 * (b - a);

    Real s = 0;
    for (int j = 0; j < 5; j++)
    {
        Real dx = xr * x[j];
        s += w[j] * (func(xm + dx) + func(xm - dx));
    }
    return s *= xr;
}
```

Examples of usage – integrating real function

https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/Chapter_02_basic_algorithms/demo_integrating.cpp

```
RealFunction f1{ [](Real x) { return (Real)(sin(x) * (1.0 + 0.5 * x * x)); } };
RealFunction f1_integral{ [](Real x) { return (Real)(x * (-0.5 * x * cos(x)) + sin(x))); } };

double a = 0.0;
double b = 10.0;
double int_trap = IntegrateTrap(f1, a, b);
double int_simp = IntegrateSimpson(f1, a, b);
double int_gauss = IntegrateGauss10(f1, a, b);

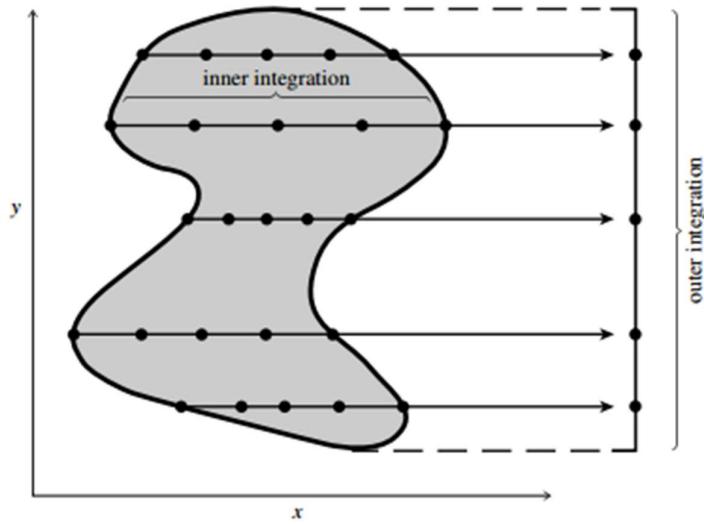
std::cout << "Integrating function f1 from " << a << " to " << b << std::endl;
std::cout << "Exact integral = " << f1_integral(b) - f1_integral(a) << std::endl;
std::cout << "IntegrateTrap = " << int_trap << std::endl;
std::cout << "IntegrateSimpson = " << int_simp << std::endl;
std::cout << "IntegrateGauss10 = " << int_gauss << std::endl;

/* OUTPUT
Integrating function f1 from 0 to 10
Exact integral = 36.51336534
IntegrateTrap = 36.51297408
IntegrateSimpson = 36.51337665
IntegrateGauss10 = 36.51336529
*/
```

Integrating in 2D

TODO – intro

This is what it means to integrate numerically in 2D.



Helper function, for integrating inner loop

```
struct SurfaceIntegralInner : public IRealFunction
{
    mutable Real _currX;
    IScalarFunction<2>& _funcToIntegrate;

    SurfaceIntegralInner(IScalarFunction<2>& func) : _funcToIntegrate(func) {}

    Real operator()(const Real y) const
    {
        VectorN<Real, 2> v{ _currX, y };
        return _funcToIntegrate(v);
    }
};
```

Helper function for outer loop

```
struct SurfaceIntegralOuter : public IRealFunction
{
    mutable SurfaceIntegralInner _fInner;

    IntegrationMethod _integrMethod;
    IScalarFunction<2>& _funcToIntegrate;

    Real(*_yRangeLow)(Real);
    Real(*_yRangeUpp)(Real);

    SurfaceIntegralOuter(IScalarFunction<2>& func, IntegrationMethod inMethod,
                        Real yy1(Real), Real yy2(Real))
        : _yRangeLow(yy1), _yRangeUpp(yy2),
          _fInner(func), _funcToIntegrate(func), _integrMethod(inMethod) { }

    // for given x, will return (ie. integrate function over Y-range)
    Real operator()(const Real x) const
    {
        _fInner._currX = x;
        switch (_integrMethod)
        {
            case SIMPSON:
                return IntegrateSimpson(_fInner, _yRangeLow(x), _yRangeUpp(x));
            // ...
            case GAUSS10:
                return IntegrateGauss10(_fInner, _yRangeLow(x), _yRangeUpp(x));
            default:
                return IntegrateTrap(_fInner, _yRangeLow(x), _yRangeUpp(x));
        }
    }
};
```

And finally, main integrator

```

static Real IntegrateSurface(IScalarFunction<2>& func, IntegrationMethod method,
                           const Real x1, const Real x2,
                           Real y1(Real), Real y2(Real))
{
    SurfaceIntegralOuter f1(func, method, y1, y2);

    switch (method)
    {
        case SIMPSON:
            return IntegrateSimpson(f1, x1, x2);
        // ...
        case GAUSS10:
            return IntegrateGauss10(f1, x1, x2);
        default:
            return IntegrateTrap(f1, x1, x2);
    }
}

```

Examples of usage – integrating in 2D

https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/Chapter_02_basic_algorithms/demo_integrating_in_2d.cpp

```

// 2D integration of constant 2D function over area (ie. we'll get the area of the surface)
ScalarFunction<2> f2([](const VectorN<Real, 2>& x) { return Real{ 1 }; });

// we integrate over circle with radius 2
Real val = Integrate2D(f2, IntegrationMethod::GAUSS10,
                       -2, 2,                                // x range
                       [](Real x) { return -sqrt(4 - x * x); }, // y range lower limit
                       [](Real x) { return sqrt(4 - x * x); }); // y range upper limit

std::cout << "Circle area = " << val << ", exact value: 4 * PI = " << 4 * Constants::PI << std::endl;

// calculate volume of half-sphere
ScalarFunction<2> f3([](const VectorN<Real, 2>& x) { return Real{ sqrt(4 - POW2(x[0]) - POW2(x[1])) }; });
Real val2 = Integrate2D(f3, IntegrationMethod::GAUSS10,
                       -2, 2,                                // x range
                       [](Real x) { return -sqrt(4 - x * x); }, // y range lower limit
                       [](Real x) { return sqrt(4 - x * x); }); // y range upper limit

std::cout << "Half-sphere volume = " << val2 << ", exact value = " << 4.0 / 6 * 8 * Constants::PI << std::endl;

/* OUTPUT
   Calc. area = 12.57211164, exact value: 4 * PI = 12.56637061
   Calc. half-sphere volume = 16.76281553, exact value = 16.75516082
*/

```

Integrating in 3D

Helper function, for innermost loop integration

```
struct VolumeIntegralInnermost : public IRealFunction
{
    mutable Real      _currX, _currY;
    IScalarFunction<3>& _funcToIntegrate;

    VolumeIntegralInnermost(IScalarFunction<3>& func)
        : _funcToIntegrate(func), _currX{ 0 }, _currY{ 0 } {}

    Real operator()(const Real z) const
    {
        VectorN<Real, 3> v{ _currX, _currY, z };
        return _funcToIntegrate(v);
    }
};
```

Inner integration

```
struct VolumeIntegralInner : public IRealFunction
{
    mutable VolumeIntegralInnermost _fInnermost;

    IScalarFunction<3>& _funcToIntegrate;

    Real(*_zRangeLow)(Real, Real);
    Real(*_zRangeUpp)(Real, Real);

    VolumeIntegralInner(IScalarFunction<3>& func,
                       Real zz1(Real, Real), Real zz2(Real, Real))
        : _zRangeLow(zz1), _zRangeUpp(zz2), _funcToIntegrate(func), _fInnermost(func) {}

    Real operator()(const Real y) const
    {
        _fInnermost._currY = y;

        return IntegrateGauss10(_fInnermost,
                               _zRangeLow(_fInnermost._currX, y),
                               _zRangeUpp(_fInnermost._currX, y));
    }
};
```

Outer integration loop

```

struct VolumeIntegralOuter : public IRealFunction
{
    mutable VolumeIntegralInner _fInner;

    IScalarFunction<3>& _funcToIntegrate;
    Real(*_yRangeLow)(Real);
    Real(*_yRangeUpp)(Real);

    VolumeIntegralOuter(IScalarFunction<3>& func, Real yy1(Real), Real yy2(Real),
                        Real z1(Real, Real), Real z2(Real, Real))
        : _yRangeLow(yy1), _yRangeUpp(yy2), _funcToIntegrate(func), _fInner(func, z1, z2)
    {
    }

    Real operator()(const Real x) const
    {
        _fInner._fInnermost._currX = x;

        return IntegrateGauss10(_fInner, _yRangeLow(x), _yRangeUpp(x));
    }
};

```

And finally, volume integrator

Sets up needed objects, and fires it all up.

```

static Real IntegrateVolume(IScalarFunction<3>& func,
                            const Real x1, const Real x2,
                            Real y1(Real), Real y2(Real),
                            Real z1(Real, Real), Real z2(Real, Real))
{
    VolumeIntegralOuter f1(func, y1, y2, z1, z2);

    return IntegrateGauss10(f1, x1, x2);
}

```

Examples of usage – integrating in 3D

https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/Chapter_02_basic_algorithms/demo_integrati on_3d.cpp

```

// 3D integration of constant scalar 3D function (ie. we'll get the volume of the solid)
ScalarFunction<3> f3([](const VectorN<Real, 3>& x) { return Real{ 1 }; });

// integration over cube with sides 2, 3, 4
Real cubeVol = Integrate3D(f3,
    -1, 1,
    [](Real x) { return -1.5; },
    [](Real x) { return 1.5; },
    [](Real x, Real y) { return -2.0; },
    [](Real x, Real y) { return 2.0; });

std::cout << "Cube vol. = " << cubeVol << ", exact value: 2 * 3 * 4 = " << 2 * 3 * 4 << std::endl;

// integration over sphere of radius 1
Real sphereVol = Integrate3D(f3,
    -1, 1,
    [] (Real x) { return -sqrt(1 - x * x); },
    [] (Real x) { return sqrt(1 - x * x); },
    [] (Real x, Real y) { return -sqrt(1 - x * x - y * y); },
    [] (Real x, Real y) { return sqrt(1 - x * x - y * y); });

std::cout << "Sphere vol. = " << sphereVol << ", exact value: 4/3*PI = " << 4.0/3*Constants::PI << std::endl;

/* OUTPUT
   Cube vol. = 24, exact value: 2 * 3 * 4 = 24
   Sphere vol. = 4.1907, exact value: 4/3 * PI = 4.18879
*/

```

INTERPOLATING FUNCTIONS

TODO – INTRO

Base class for interpolating real functions

<https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/mml/base/InterpolatedFunction.h>

```
class RealFunctionInterpolated : public IRealFunction
{
private:
    int _numPoints, _usedPoints;
    Vector<Real> _x, _y;           // we are storing copies of given values!

public:
    RealFunctionInterpolated(const Vector<Real> &x, const Vector<Real> &y,
                           int usedPointsInInterpolation)
        : _x(x), _y(y), _numPoints(x.size()), _usedPoints(usedPointsInInterpolation)
    {
        // throw if not enough points
        if (_numPoints < 2 || _usedPoints < 2 || _usedPoints > _numPoints)
            throw RealFuncInterpInitError("RealFunctionInterpolated size error");
    }

    virtual ~RealFunctionInterpolated() {}

    Real virtual calcInterpValue(int startInd, Real x) const = 0;

    inline Real MinX() const { return X(0); }
    inline Real MaxX() const { return X(_numPoints-1); }

    inline Real X(int i) const { return _x[i]; }
    inline Real Y(int i) const { return _y[i]; }

    inline int getNumPoints() const { return _numPoints; }
    inline int getInterpOrder() const { return _usedPoints; }

    Real operator()(Real x) const
    {
        int startInd = locate(x);
        return calcInterpValue(startInd, x);
    }

    // Given a value x, return a value j such that x is (insofar as possible) centered in the subrange
    // xx[j..j+mm-1], where xx is the stored pointer. The values in xx must be monotonic, either
    // increasing or decreasing. The returned value is not less than 0, nor greater than _numPoints-1.
    int locate(const Real x) const { ... }
};
```

LinearInterpRealFunc

```
class LinearInterpRealFunc : public RealFunctionInterpolated
{
public:
    LinearInterpRealFunc(const Vector<Real>& xv, Vector<Real>& yv)
        : RealFunctionInterpolated(xv, yv, 2) {}

    Real calcInterpValue(int j, Real x) const {
        if (X(j) == X(j + 1))
            return Y(j);
        else
            return Y(j) + ((x - X(j)) / (X(j + 1) - X(j)) * (Y(j + 1) - Y(j)));
    }
};
```

PolynomInterpFunc

```
// Polynomial interpolation object. Construct with x and y vectors, and the number M of points
// to be used locally(polynomial order plus one), then call interp for interpolated values.
class PolynomInterpRealFunc : public RealFunctionInterpolated
{
private:
    mutable Real _errorEst;
public:
    PolynomInterpRealFunc(const Vector<Real>& xv, Vector<Real>& yv, int m)
        : RealFunctionInterpolated(xv, yv, m), _errorEst(0.) {}

    Real getLastErrorEst() const { return _errorEst; }

    // Given a value x, and using pointers to data xx and yy, this routine returns an interpolated
    // value y, and stores an error estimate _errorEst. The returned value is obtained by mm-point polynomial
    // interpolation on the subrange xx[startInd..startInd + mm - 1].
    Real calcInterpValue(int startInd, Real x) const[...]
};
```

SplineInterpFunc

```
// Cubic spline interpolation object. Construct with x and y vectors, and (optionally) values of
// the first derivative at the endpoints, then call interp for interpolated values.
struct SplineInterpRealFunc : RealFunctionInterpolated
{
    Vector<Real> _secDerY;

    SplineInterpRealFunc(Vector<Real>& xv, Vector<Real>& yv, Real ypl = 1.e99, Real ypn = 1.e99)
        : RealFunctionInterpolated(xv, yv, 2), _secDerY(xv.size())
    {
        initSecDerivs(&xv[0], &yv[0], ypl, ypn);
    }

    // This routine stores an array _secDerY[0..numPoints-1] with second derivatives of the interpolating function
    // at the tabulated points pointed to by xv, using function values pointed to by yv. If ypl and/or
    // ypn are equal to 1 1099 or larger, the routine is signaled to set the corresponding boundary
    // condition for a natural spline, with zero second derivative on that boundary; otherwise, they are
    // the values of the first derivatives at the endpoints.
    void initSecDerivs(const Real* xv, const Real* yv, Real ypl, Real ypn)[...]

    // Given a value x, and using pointers to data xx and yy, and the stored vector of second derivatives
    // _secDerY, this routine returns the cubic spline interpolated value y.
    Real calcInterpValue(int startInd, Real x) const[...]
};
```

ParametricCurveSplineInterp

Using SplineInterpFunc objects, constructs cubic spline interpolation for parametric curve in N dimension.

```
// Object for interpolating a curve specified by _numPoints points in N dimensions.
template<int N>
class SplineInterpParametricCurve : public IParametricCurve<N>
{
    Real _minT, _maxT;
    int _dim, _numPoints, _bemba;
    bool _isCurveClosed;

    Matrix<Real> _curvePoints;
    Vector<Real> s;
    Vector<Real> ans;

    std::vector<SplineInterpRealFunc*> srp;

public:
    // Constructor. The _numPoints _dim matrix ptsin inputs the data points. Input close as 0 for
    // an open curve, 1 for a closed curve. (For a closed curve, the last data point should not
    // duplicate the first - the algorithm will connect them.)
    SplineInterpParametricCurve(Real minT, Real maxT, const Matrix<Real>& ptsin, bool close = 0) { ... }

    SplineInterpParametricCurve(const Matrix<Real>& ptsin, bool close = 0) { ... }

    ~SplineInterpParametricCurve() { ... }

    Real getMinT() const { return _minT; }
    Real getMaxT() const { return _maxT; }

    // Interpolate a point on the stored curve. The point is parameterized by t, in the range [0,1].
    // For open curves, values of t outside this range will return extrapolations (dangerous!). For
    // closed curves, t is periodic with period 1
    VectorN<Real, N> operator()(Real t) const { ... }

    // ...
    Real fprime(Real* x, Real* y, int pm) { ... }

    Real rad(const Real* p1, const Real* p2) { ... }
};
```

Example usage – interpolating functions

https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/Chapter_02_basic_algorithms/demo_interpolation.cpp

```

// we are manually creating data for interpolation in two vectors
// but generally you would have some data from some source
Real x1 = 0.0;
Real x2 = 10.0;
Vector<Real> vec_x{ 0.0, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0 };
Vector<Real> vec_y{ 0.0, 1.0, 4.0, -2.0, -16, -13, 6, 6.2, 5.5, 12.0, 3.0 };

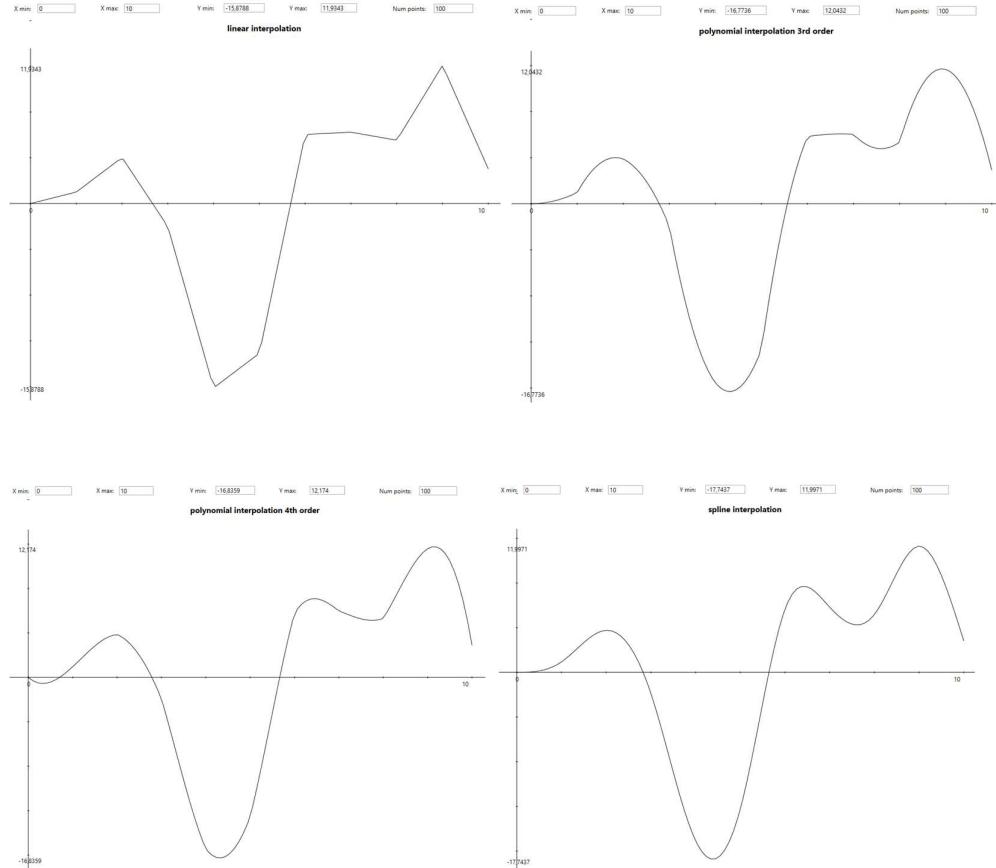
// create InterpolatedFunction object
LinearInterpRealFunc lin_interp(vec_x, vec_y);
PolynomInterpRealFunc poly_interp3(vec_x, vec_y, 3);
PolynomInterpRealFunc poly_interp4(vec_x, vec_y, 4);
SplineInterpRealFunc spline_interp(vec_x, vec_y);

// visualize interpolations
Visualizer::VisualizeRealFunction(lin_interp, "linear interpolation",
                                  x1, x2, 100, "example2_lin_interp.txt");
Visualizer::VisualizeRealFunction(poly_interp3, "polynomial interpolation 3rd order",
                                  x1, x2, 100, "example2_poly_interp3.txt");
Visualizer::VisualizeRealFunction(poly_interp4, "polynomial interpolation 4th order",
                                  x1, x2, 100, "example2_poly_interp4.txt");
Visualizer::VisualizeRealFunction(spline_interp, "spline interpolation",
                                  x1, x2, 100, "example2_spline_interp.txt");

// visualize all together
Visualizer::VisualizeMultiRealFunction({&lin_interp, &poly_interp3, &poly_interp4, &spline_interp},
                                       "Interpolation comparison",
                                       0.0, 10.0, 100, "example2_interpolation.txt" );

```

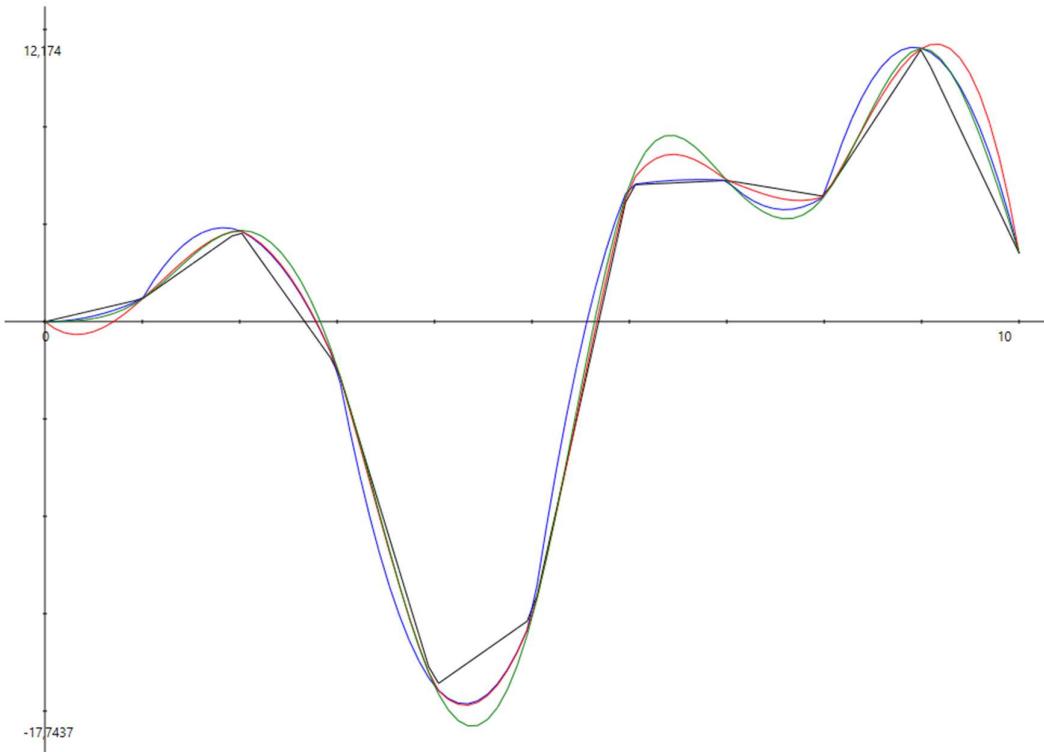
Visualizations



All together.

X min: X max: Y min: Y max: Num points:

Interpolation comparison



ROOT FINDING

Analytically finding roots of functions is possible in a very limited set of cases.

Polynomial roots up to 4th order

We can use functions from MMLBase.h

```
// a * x^2 + b * x + c = 0
static int SolveQuadratic(Real a, Real b, Real c,
                           Complex& x1, Complex& x2) { ... }

static void SolveQuadratic(const Complex &a, const Complex &b, const Complex &c,
                           Complex& x1, Complex& x2) { ... }

// CHECK!!!
static void SolveCubic(Real a, Real b, Real c, Real d,
                       Complex& x1, Complex& x2, Complex& x3) { ... }

// TODO!!!
static void SolveQuartic(Real a, Real b, Real c, Real d, Real e,
                        Complex& x1, Complex& x2, Complex& x3, Complex& x4) { ... }
```

And we mostly have to rely on numerical methods.

Bracketing roots

Two functions that help with bracketing roots.

```
// Given a function func and an initial guessed range x1 to x2, the routine expands
// the range geometrically until a root is bracketed by the returned values x1 and x2 (in which
// case function returns true) or until the range becomes unacceptably large (in which case we
// return false).
static bool BracketRoot(const IRealFunction& func, double& x1, double& x2, int MaxTry = 50) { ... }

// Given a function fx defined on the interval[x1, x2], subdivide the interval into
// _numPoints equally spaced segments, and search for zero crossings of the function._numRoots will be set
// to the number of bracketing pairs found. If it is positive, the vectors xb1[0.._numRoots - 1] and
// xb2[0.._numRoots - 1] will be filled sequentially with any bracketing pairs that are found. On input,
// these vectors may have any size, including zero; they will be resized to _numRoots.
static void FindRootBrackets(const IRealFunction& func, const Real x1, const Real x2, const int numPoints,
                             Vector<Real>& xb1, Vector<Real>& xb2, int& numRoots) { ... }
```

Bisection

```
// Using bisection, return the root of a function or functor func known to lie between x1 and x2.
// The root will be refined until its accuracy is xacc.
static Real FindRootBisection(const IRealFunction& func, Real x1, Real x2, Real xacc) { ... }
```

Newton-Raphson algorithm

```
// Using the Newton-Raphson method, return the root of a function known to lie in the interval
// x1; x2. The root will be refined until its accuracy is known within 'xacc'.
static Real FindRootNewton(const IRealFunction& func, Real x1, Real x2, Real xacc)
{
    Real rtn = 0.5 * (x1 + x2);
    for (int j = 0; j < Defaults::NewtonRaphsonMaxSteps; j++)
    {
        Real f  = func(rtn);
        Real df = Derivation::NDer4(func, rtn);

        Real dx = f / df;

        rtn -= dx;

        if ((x1 - rtn) * (rtn - x2) < 0.0)
            throw RootFindingError("Jumped out of brackets in FindRootNewton");

        if (std::abs(dx) < xacc)
            return rtn;
    }
    throw RootFindingError("Maximum number of iterations exceeded in FindRootNewton");
}
```

Example usage – root finding

https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/Chapter_02_basic_algorithms/demo_root_finding.cpp

Simple example of finding (single) root of a function.

```
// Finding the root of the function f(x) = x^2 - 2
// (with known root sqrt(2) = 1.414213562373095)
RealFunction f{ [](Real x) { return x * x - 2; } };
Real a = 0.0;
Real b = 10.0;

Real root = FindRootBisection(f, a, b, 0.0001);

std::cout << "Root of the function using the bisection method: " << root << std::endl;
std::cout << "Exact root: " << sqrt(2) << std::endl;
std::cout << "Error: " << abs(root - sqrt(2)) << std::endl;
```

Example with function with multiple roots.

```
Real x1 = -20.0;
Real x2 = 20.0;
RealFunction f2{ [](Real x) { return x * x * sin(x) * exp(2-Abs(x/2)); } };

int numFoundRoots;
Vector<Real> root_brack_x1(10), root_brack_x2(10);
FindRootBrackets(f2, x1, x2, 100, root_brack_x1, root_brack_x2, numFoundRoots);

std::cout << "Number of found roots: " << numFoundRoots << std::endl;

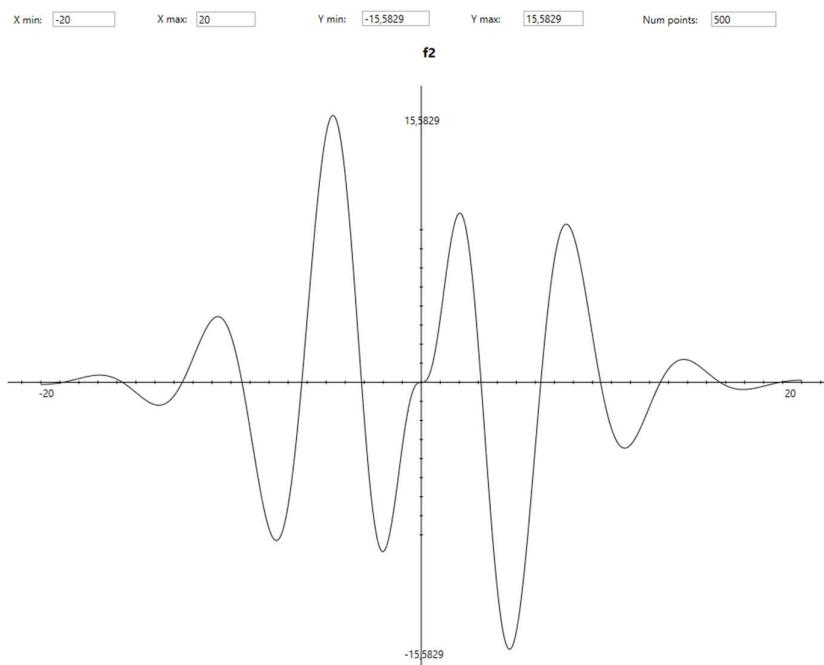
Vector<Real> roots(numFoundRoots);
for (int i = 0; i < numFoundRoots; i++)
{
    roots[i] = FindRootBisection(f2, root_brack_x1[i], root_brack_x2[i], 1e-7);

    std::cout << "Root " << i << " : " << roots[i] << std::endl;
}

// visualize the function
Visualizer::VisualizeRealFunction(f2, "f2", x1, x2, 500, "example2_root_finding.txt");
```

Program output and function visualization.

```
Number of found roots: 13
Root 0 : -18.8496
Root 1 : -15.708
Root 2 : -12.5664
Root 3 : -9.42478
Root 4 : -6.28319
Root 5 : -3.14159
Root 6 : -4.10783e-15
Root 7 : 3.14159
Root 8 : 6.28319
Root 9 : 9.42478
Root 10 : 12.5664
Root 11 : 15.708
Root 12 : 18.8496
```



4. From colliding mechanical balls to gas laws

Embarking on our journey with some 17th and 18th century physics.

Tasks at hand:

- Given positions and initial velocities of N simple mechanical balls, confined to 2D or 3D container, calculate their positions in time.
- Relate to gas laws

PHYSICS OF COLLIDING MECHANICAL BALLS

Starting with basics of physics

We'll need First and Third Newton law (but not the Second!), and law of conservation of energy together with law of conservation of momentum.

One-dimensional case

TODO - Two balls, pictured on a line.

Conservation of momentum:

$$m_A v_{A1} + m_B v_{B1} = m_A v_{A2} + m_B v_{B2}.$$

Conservation of energy:

$$\frac{1}{2} m_A v_{A1}^2 + \frac{1}{2} m_B v_{B1}^2 = \frac{1}{2} m_A v_{A2}^2 + \frac{1}{2} m_B v_{B2}^2.$$

When solved, gives:

$$\begin{aligned} v_{A2} &= \frac{m_A - m_B}{m_A + m_B} v_{A1} + \frac{2m_B}{m_A + m_B} v_{B1} \\ v_{B2} &= \frac{2m_A}{m_A + m_B} v_{A1} + \frac{m_B - m_A}{m_A + m_B} v_{B1}. \end{aligned}$$

Center of mass frame doesn't change!

Two-dimensional case

Dependent on the point of collision, and after lengthy calculation, in an angle-free representation, the changed velocities are computed using the centers \mathbf{x}_1 and \mathbf{x}_2 at the time of contact as:

$$\begin{aligned}\mathbf{v}'_1 &= \mathbf{v}_1 - \frac{2m_2}{m_1 + m_2} \frac{\langle \mathbf{v}_1 - \mathbf{v}_2, \mathbf{x}_1 - \mathbf{x}_2 \rangle}{\|\mathbf{x}_1 - \mathbf{x}_2\|^2} (\mathbf{x}_1 - \mathbf{x}_2), \\ \mathbf{v}'_2 &= \mathbf{v}_2 - \frac{2m_1}{m_1 + m_2} \frac{\langle \mathbf{v}_2 - \mathbf{v}_1, \mathbf{x}_2 - \mathbf{x}_1 \rangle}{\|\mathbf{x}_2 - \mathbf{x}_1\|^2} (\mathbf{x}_2 - \mathbf{x}_1)\end{aligned}$$

Based on these equations, we can easily implement calculations of velocity vectors for two balls after collision:

```
Vec2Cart v1 = ball1.V(), v2 = ball2.V();

Vec2Cart v1_v2 = v1 - v2;
Vec2Cart x1_x2(x2, x1);

Vec2Cart v1_new = v1 - 2 * m2 / (m1 + m2) * (v1_v2 * x1_x2) / POW2(x1_x2.NormL2()) * Vec2Cart(x2, x1);
Vec2Cart v2_new = v2 - 2 * m1 / (m1 + m2) * (v1_v2 * x1_x2) / POW2(x1_x2.NormL2()) * Vec2Cart(x1, x2);
```

DOING A 2D SIMULATION - COLLISIONSIMULATOR2D

Building a simple collision simulator.

https://github.com/zvanjak/ExploringPhysicsWithCpp/blob/master/Code/Chapter_04_collision_simulator/collision_simulator_2d.cpp

Starting with a model of 2D ball.

```
struct Ball2D
{
private:
    double _mass;
    double _radius;
    Point2Cartesian _position;
    Vector2Cartesian _velocity;

public:
    Ball2D(double mass, double radius, const Point2Cartesian& position,
           const Vector2Cartesian& velocity) { ... }

    double Mass() const { return _mass; }
    double& Mass() { return _mass; }

    double Rad() const { return _radius; }
    double& Rad() { return _radius; }

    Point2Cartesian Pos() const { return _position; }
    Point2Cartesian& Pos() { return _position; }

    Vector2Cartesian V() const { return _velocity; }
    Vector2Cartesian& V() { return _velocity; }
};
```

Container for our balls.

Simple rectangle, with bottom left corner at point (0,0), with given width and height.

```
struct Container2D
{
    double _width;
    double _height;

    std::vector<Ball2D> _balls;

    Container2D() : _width(1000), _height(1000) {}
    Container2D(double width, double height) : _width(width), _height(height) {}

    // add body
    void AddBall(const Ball2D& body) { ... }

    // get body
    Ball2D& Ball(int i) { ... }

    // check if ball is out of bounds and handle it
    void CheckAndHandleOutOfBounds(int ballIndex) { ... }
};
```

Where CheckAndHandleOutOfBounds() function is crucial:

```
void CheckAndHandleOutOfBounds(int ballIndex)
{
    const Ball2D& ball = ball;

    // left wall collision
    if (ball.Pos().X() < ball.Rad() && ball.V().X() < 0)
    {
        ball.Pos().X() = ball.Rad() + (ball.Rad() - ball.Pos().X()); // Get back to box!
        ball.V().X() *= -1;
    }
    // right wall collision
    if (ball.Pos().X() > _width - ball.Rad() && ball.V().X() > 0)
    {
        ball.Pos().X() -= (ball.Pos().X() + ball.Rad()) - _width;
        ball.V().X() *= -1;
    }
    // bottom wall collision
    if (ball.Pos().Y() < ball.Rad() && ball.V().Y() < 0)
    {
        ball.Pos().Y() = ball.Rad() + (ball.Rad() - ball.Pos().Y());
        ball.V().Y() *= -1;
    }
    // top wall collision
    if (ball.Pos().Y() > _height - ball.Rad() && ball.V().Y() > 0)
    {
        ball.Pos().Y() -= (ball.Pos().Y() + ball.Rad()) - _height;
        ball.V().Y() *= -1;
    }
}
```

And finally, CollisionSimulator2D class, implementing simulator.

```
class CollisionSimulator2D
{
    Container2D _box;

public:
    CollisionSimulator2D() { }
    CollisionSimulator2D(const Container2D& box) : _box(box) {}

    double DistBalls(int i, int j){ ... }

    bool HasBallsCollided(int i, int j){ ... }

    void SimulateOneStep(double dt){ ... }

    void HandleCollision(int m, int n, double dt){ ... }

    std::vector<std::vector<Pnt2Cart>> Simulate(int numSteps, double timeStep){ ... }

    void Serialize(std::string fileName, std::vector<std::vector<Pnt2Cart>> ballPositions){ ... };
};
```

HandleCollision is the most important function here.

```
void HandleCollision(int m, int n, double dt)
{
    Ball2D& ball1 = _box._balls[m];
    Ball2D& ball2 = _box._balls[n];

    // calculating point where they were before collision
    // (if there was collision with the box wall, then calc.pos. will be outside the box
    // but it doesn't matter, since we need only direction, ie. velocity, to calculate exact collision point)
    Pnt2Cart x10 = ball1.Pos() - ball1.V() * dt;
    Pnt2Cart x20 = ball2.Pos() - ball2.V() * dt;

    Vec2Cart dx0(x10, x20);
    Vec2Cart dv(ball2.V() - ball1.V());

    // first, we have to calculate exact moment of collision, and balls positions then
    double A = dv * dv;
    double B = 2 * dx0 * dv;
    double C = dx0 * dx0 - POW2(ball2.Rad() + ball1.Rad());

    double t1 = (-B + sqrt(B * B - 4 * A * C)) / (2 * A);
    double t2 = (-B - sqrt(B * B - 4 * A * C)) / (2 * A);

    double tCollision = t1 < t2 ? t1 : t2;
```

```

// calculating position of balls at the point of collision (moving them backwards)
Pnt2Cart x1 = ball1.Pos() + (tCollision - dt) * ball1.V();
Pnt2Cart x2 = ball2.Pos() + (tCollision - dt) * ball2.V();

// https://en.wikipedia.org/wiki/Elastic\_collision - calculating new velocities after collision
double m1 = ball1.Mass(), m2 = ball2.Mass();

Vec2Cart v1 = ball1.V(), v2 = ball2.V();

Vec2Cart v1_v2 = v1 - v2;
Vec2Cart x1_x2(x2, x1);

Vec2Cart v1_new = v1 - 2 * m2 / (m1 + m2) * (v1_v2 * x1_x2) / POW2(x1_x2.NormL2()) * Vec2Cart(x2, x1);
Vec2Cart v2_new = v2 - 2 * m1 / (m1 + m2) * (v1_v2 * x1_x2) / POW2(x1_x2.NormL2()) * Vec2Cart(x1, x2);

ball1.V() = v1_new;
ball2.V() = v2_new;

// adjusting new ball positions
ball1.Pos() = x1 + ball1.V() * (dt - tCollision);
ball2.Pos() = x2 + ball2.V() * (dt - tCollision);
}

```

3D SIMULATION

Implementation is the same, only using Vector3Cartesian in CollisionSiulator3D class.

And of course, we need Container3D, and there is the only non-trivial functions to be added – CheckAndHandleOutOfBonds() for 3D case, which looks like this:

```

void CheckAndHandleOutOfBounds(int ballIndex)
{
    Ball3D& ball = _balls[ballIndex];

    if (ball.Pos().X() < ball.Rad() && ball.V().X() < 0)      // checking if ball is out of bounds
    {
        ball.Pos().X() = ball.Rad() + (ball.Rad() - ball.Pos().X());      // moving it back to box
        ball.V().X() *= -1;
    }

    if (ball.Pos().X() > _width - ball.Rad() && ball.V().X() > 0)
    {
        ball.Pos().X() -= (ball.Pos().X() + ball.Rad()) - _width;
        ball.V().X() *= -1;
    }

    if (ball.Pos().Y() < ball.Rad() && ball.V().Y() < 0)
    {
        ball.Pos().Y() = ball.Rad() + (ball.Rad() - ball.Pos().Y());
        ball.V().Y() *= -1;
    }

    if (ball.Pos().Y() > _height - ball.Rad() && ball.V().Y() > 0)
    {
        ball.Pos().Y() -= (ball.Pos().Y() + ball.Rad()) - _height;
        ball.V().Y() *= -1;
    }

    if (ball.Pos().Z() < ball.Rad() && ball.V().Z() < 0)
    {
        ball.Pos().Z() = ball.Rad() + (ball.Rad() - ball.Pos().Z());
        ball.V().Z() *= -1;
    }

    if (ball.Pos().Z() > _depth - ball.Rad() && ball.V().Z() > 0)
    {
        ball.Pos().Z() -= (ball.Pos().Z() + ball.Rad()) - _depth;
        ball.V().Z() *= -1;
    }
}

```

Visualizing with WPF

Visualizing container with balls with Qt

TODO

PHYSICS – IDEAL GAS

Model of colliding balls in elastic collision is fairly good approximation for ideal gas.

Little bit of formulas.

SIMULATING IDEAL GAS

Developed collision simulator can be used to verify basic gas laws, as our mechanical balls model represents most of the ideal gas approximations.

Calculating pressure by summing momentum transferred to walls during collisions

Calculating temperature from average kinetic energy of balls

Verifying $pV = nRT$ gas equation

PISTON SIMULATION

Cylinder with movable wall in the middle

What happens if we inject highly energetic balls into one side?

Could we simulate chemical reactions?

- When different types of “molecules” collide, there is released energy, which translates to higher velocities after “collision”

IMPROVING EFFICIENCY FOR LARGE NUMBER OF BALLS

Implemented algorithm scales as $O(N^2)$!

Feasible for under 1000 balls.

What can we do if we want to simulate one million balls?

5. Pendulum - Newton laws and ODE solvers

Introducing forces ... and the emperors of numerical simulations, ODE solvers.

Tasks at hand:

- Introduce pendulum as one of the simplest physical systems
- Introduce numerical ODE solvers and solve exactly motion of pendulum
- Compare obtained solutions with analytical one
- What if we add air resistance?

PHYSICS OF PENDULUM

TODO – intro to pendulum

FORCES!!! Second Newton law.

Applying Newton second law to tangential component, we get

$$F = -mg \sin \theta = ma, \\ a = -g \sin \theta, \quad (5.1)$$

The negative sign on the right-hand side means that θ and a always point in opposite directions

This linear acceleration a along the red axis can be related to the change in angle θ by the arc length formulas; s is arc length:

$$s = \ell\theta, \\ v = \frac{ds}{dt} = \ell \frac{d\theta}{dt}, \\ a = \frac{d^2 s}{dt^2} = \ell \frac{d^2 \theta}{dt^2},$$

Inserting this into equation 5.1, we get

$$\ell \frac{d^2 \theta}{dt^2} = -g \sin \theta,$$

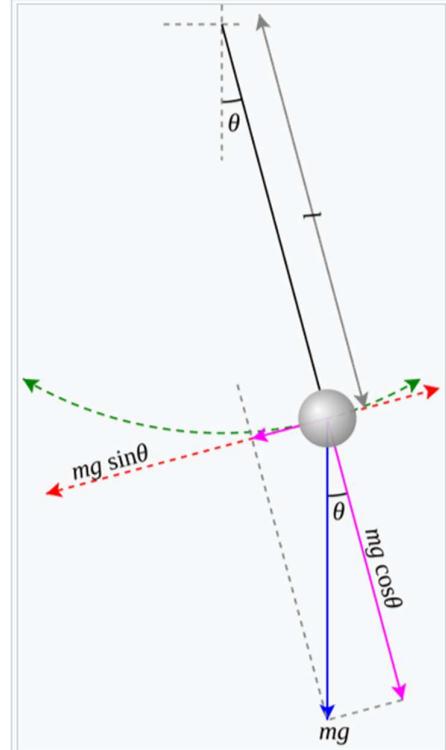


Figure 1. Force diagram of a simple gravity pendulum.

Picture from Wikipedia.

Giving us our final exact equation of motion for simple pendulum:

$$\frac{d^2\theta}{dt^2} + \frac{g}{\ell} \sin \theta = 0.$$

Exact solution involves elliptic integrals (more on that a little bit later), but we can employ linear approximation for small angles ($\theta \ll 1$), where we approximate $\sin \theta \approx \theta$, which gives as an equation for harmonic oscillator, that is a linear differential equation of second order.

$$\frac{d^2\theta}{dt^2} + \frac{g}{\ell} \theta = 0.$$

Solution for dependence of angle on time, if we assume initial angle θ_0 , is given by:

$$\theta(t) = \theta_0 \cos\left(\sqrt{\frac{g}{\ell}} t\right) \quad \theta_0 \ll 1.$$

With period of motion given by one of the most famous equations of high-school physics:

$$T_0 = 2\pi \sqrt{\frac{\ell}{g}}$$

How can we calculate exact values?

Elliptic integrals come to play ...

SOLVING ODEs NUMERICALLY

When numerically solving differential equations, it is always possible to reduce them to a set of coupled *first-order* ODE's. For example, the second-order equation

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

Can be reduced to a system of two first-order equations

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

With introduction of new variable $z(x)$.

Therefore, all numerical solvers are aimed at solving a set of N first-order equations for functions y_i , $i = 0, \dots, N-1$, with the general form:

$$\frac{dy_i(x)}{dx} = f_i(x, y_0, \dots, y_{N-1}), \quad i = 0, \dots, N-1$$

Importance of initial conditions

- Initial-value problems
- Boundary-value problems

Euler method

Formula for Euler method:

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

Midpoint method

Formula:

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

Runge-Kutta methods

Formula:

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

Adaptive step size methods

Richardson extrapolation (Bulirsch-Stoer)

Predictor-corrector multi-step methods

IMPLEMENTING ODE SOLVERS IN C++

First question is – how to model system of ODE's?

ODESystem class

Basic interface, used for modelling system of ordinary differential equations.

```
class IODESystem
{
public:
    virtual int    getDim() const = 0;
    virtual void   derivs(const Real t, const Vector<Real> &x, Vector<Real> &dxdt) const = 0;
};
```

You can use it to create your own ODE system, by inheriting this interface in your class and providing two virtual methods.

TODO – example ODE from introduction, but for now, Pendulum example from chapter 5 will do.

```
class PendulumODE : public IODESystem
{
    Real _Length;
public:
    PendulumODE(Real length) : _Length(length) {}

    int    getDim() const override { return 2; }
    void   derivs(const Real t, const MML::Vector<Real> &x, MML::Vector<Real> &dxdt) const override
    {
        dxdt[0] = x[1];
        dxdt[1] = -9.81 / _Length * sin(x[0]);
    }
};
```

If you already have a (static) function ready with derivatives calculation, or maybe your system equations can be easily coded with simple lambda, you can use provided ODESSystem class.

```
class ODESSystem : public IODESystem
{
protected:
    int _dim;
    void (*_func)(Real, const Vector<Real>&, Vector<Real>&);

public:
    ODESSystem() : _dim(0), _func(nullptr) { }
    ODESSystem(int n, void (*inFunc)(Real, const Vector<Real>&, Vector<Real>&))
        : _dim(n), _func(inFunc) { }

    int getDim() const { return _dim; }
    void derivs(const Real x, const Vector<Real>& y, Vector<Real>& dydx) const { ... }
};
```

Example of pendulum system definition using lambda.

```
void Demo_ExactPendulum()
{
    ODESSystem pendSys(2, [](Real t, const Vector<Real>& x, Vector<Real>& dxdt)
    {
        Real Length = 1.0;
        dxdt[0] = x[1];
        dxdt[1] = -9.81 / Length * sin(x[0]);
    });
}
```

Created object pendSys is ready to be supplied wherever IODESystem reference is expected.

Important thing to note is that in case with lambda definition, Length parameter is hard-coded within lambda, and can't be changed in run-time!

ODESystemSolution class

For storing our calculation results.

```
class ODESSystemSolution
{
    int _numStepsOK, _numStepsBad;

    int _sys_dim;
    int _totalSavedSteps;

    Real _t1, _t2;
    Vector<Real> _tval;
    Matrix<Real> _xval;

public:
    ODESSystemSolution(Real x1, Real x2, int dim) { ... }
    ODESSystemSolution(Real x1, Real x2, int dim, int maxSteps) { ... }
```

Public functions.

```
void incrementNumStepsOK() { _numStepsOK++; }
void incrementNumStepsBad() { _numStepsBad++; }

int getSysDym() const { return _sys_dim; }
int getNumStepsOK() const { return _numStepsOK; }
int getNumStepsBad() const { return _numStepsBad; }
int getTotalNumSteps() const { return _numStepsOK + _numStepsBad; }

Vector<Real> getTValues() const { return _tval; }
Matrix<Real> getXValues() const { return _xval; }
Vector<Real> getXValues(int component) const { ... }

void fillValues(int ind, Real x, Vector<Real>& y) { ... }
void setFinalSize(int numDoneSteps) { ... }

LinearInterpRealFunc getSolutionAsLinearInterp(int component) const { ... }
PolynomInterpRealFunc getSolutionAsPolyInterp(int component, int polyOrder) const { ... }
SplineInterpRealFunc getSolutionAsSplineInterp(int component) const { ... }

bool Serialize(std::string fileName, std::string title) const { ... }
bool SerializeAsParametricCurve3D(std::string fileName, std::string title) const { ... }
```

Step calculators

Have interface defined in IODESystemStepCalculators.h

```
class IODESystemStepCalculator
{
public:
    virtual void calcStep(const IODESystem& odeSystem,
                          const Real x, const Vector<Real>& y_start, const Vector<Real>& dydx,
                          const Real h, Vector<Real>& yout, Vector<Real>& yerr) const = 0;
};
```

Euler

```
class EulerStep_Calculator : public IODESystemStepCalculator
{
public:
    // For a given IODESystem of dimension n, and given initial values for the variables x_start[0..n-1]
    // and their derivatives dxdt[0..n-1] known at t, uses the Euler method to advance the solution
    // over an interval h and return the incremented variables as x_out[0..n-1].
    void calcStep(const IODESystem& odeSystem,
                  const Real t, const Vector<Real>& x_start, const Vector<Real>& dxdt,
                  const Real h, Vector<Real>& x_out, Vector<Real>& x_err_out) const override
    {
        int i, n = odeSystem.getDim();
        for (i = 0; i < n; i++)
            x_out[i] = x_start[i] + h * dxdt[i];
    }
};
```

Midpoint

```
class MidpointStep_Calculator : public IODESystemStepCalculator
{
public:
    // ...
    void calcStep(const IODESystem& odeSystem,
                  const Real t, const Vector<Real>& x_start, const Vector<Real>& dxdt,
                  const Real h, Vector<Real>& x_out, Vector<Real>& x_err_out) const override
    {
        int i, n = odeSystem.getDim();
        Vector<Real> x_mid(n);

        for (i = 0; i < n; i++)
            x_mid[i] = x_start[i] + 0.5 * h * dxdt[i];

        odeSystem.derivs(t + 0.5 * h, x_mid, x_out);
    }
};
```

Basic RK4

```
class RK4_FixedStep_Calculator : public IODESystemStepCalculator
{
public:
    // For a given ODESystem, of dimension n, and given values for the variables y_start[0..n-1]
    // and their derivatives dydx[0..n-1] known at x, uses the fourth-order Runge-Kutta method
    // to advance the solution over an interval h and return the incremented variables as yout[0..n-1].
    void calcStep(const IODESystem& odeSystem,
                  const Real t, const Vector<Real> &x_start, const Vector<Real> &dxdt,
                  const Real h, Vector<Real> &x_out, Vector<Real> &x_err_out) const override
    {
        int i, n = odeSystem.getDim();
        Vector<Real> dx_mid(n), dx_temp(n), x_temp(n);

        Real xh, hh, h6;
        hh = h * 0.5;
        h6 = h / 6.0;
        xh = t + hh;

        for (i = 0; i < n; i++)                                // First step
            x_temp[i] = x_start[i] + hh * dxdt[i];

        odeSystem.derivs(xh, x_temp, dx_temp);                // Second step

        for (i = 0; i < n; i++)
            x_temp[i] = x_start[i] + hh * dx_temp[i];

        odeSystem.derivs(xh, x_temp, dx_mid);                 // Third step

        for (i = 0; i < n; i++) {
            x_temp[i] = x_start[i] + h * dx_mid[i];
            dx_mid[i] += dx_temp[i];
        }

        odeSystem.derivs(t + h, x_temp, dx_temp);              // Fourth step

        for (i = 0; i < n; i++)
            x_out[i] = x_start[i] + h6 * (dxdt[i] + dx_temp[i] + 2.0 * dx_mid[i]);
    }
};
```

Fixed-step ODE solver

For a given ODESolver and StepCalculator, performs integration of ODESolver with a given number of fixed-size steps.

```
class ODESolverFixedStepSolver
{
    IODESystem& _odeSys;
    IODESystemStepCalculator& _stepCalc;

public:
    ODESolverFixedStepSolver(IODESystem& inOdeSys, IODESystemStepCalculator& inStepCalc)
        : _odeSys(inOdeSys), _stepCalc(inStepCalc) { }

    // For given numSteps, ODESolverSolution will have numSteps+1 values!
    ODESolverSolution integrate(const Vector<Real>& initCond, Real x1, Real x2, int numSteps)
    {
        int dim = _odeSys.getDim();

        ODESolverSolution sol(x1, x2, dim, numSteps);
        Vector<Real> y(initCond), y_out(dim), dydx(dim), y_err(dim);

        sol.fillValues(0, x1, y);

        Real x = x1;
        Real h = (x2 - x1) / numSteps;

        for (int k = 1; k <= numSteps; k++) {
            _odeSys.derivs(x, y, dydx);

            _stepCalc.calcStep(_odeSys, x, y, dydx, h, y_out, y_err);

            x += h;

            y = y_out;
            sol.fillValues(k, x, y);
        }

        return sol;
    }
};
```

Implementing adaptive step ODE solver

Base stepper

```
class StepperBase {
public:
    // references that stepper gets from the solver
    IODESystem& _sys;

    Real& _t;
    Vector<Real>& _x;
    Vector<Real>& _dxdt;

    Real _absTol, _relTol;
    Real _eps;

    Real _told;

    Real _hDone, _hNext;

    Vector<Real> _xout, _xerr;

public:
    StepperBase(IODESystem& sys, Real& t, Vector<Real>& x, Vector<Real>& dxdt)
        : _sys(sys), _t(t), _x(x), _dxdt(dxdt) {
    }

    virtual void doStep(Real htry, Real eps) = 0;

    void setHDone(Real h) { _hDone = h; }
    void setHNext(Real h) { _hNext = h; }
};
```

Runge-Kutta 5th order Cash-Karp adaptive size algorithm

Example of simple adaptive size algorithm

5th order algorithm that uses embedded 4th order method to evaluate accuracy

```
class RK4_CashKarp_Stepper : public StepperBase
{
private:
    RK4_CashKarp_Calculator _stepCalc;

public:
    RK4_CashKarp_Stepper(IODESystem& sys, Real& t, Vector<Real>& x, Vector<Real>& dxdt)
        : StepperBase(sys, t, x, dxdt) {}

    /*
    Fifth-order Runge-Kutta step with monitoring of local truncation error to ensure accuracy and
    adjust stepsize. Input are the dependent variable vector y[1..._numPoints] and its derivative dydx[1..._numPoints]
    at the starting value of the independent variable x. Also input are the stepsize to be attempted
    htry, the required accuracy eps,
    On output, y and x are replaced by their new values, hdid is the stepsize that was
    actually accomplished, and hnxt is the estimated next stepsize. derivs is the user-supplied
    routine that computes the right-hand side derivatives.
    */
    void doStep(Real htry, Real eps) override { ... }
};
```

Adaptive step calculation

```
void doStep(Real htry, Real eps) override
{
    const Real SAFETY = 0.9, PGROW = -0.2, PSHRNK = -0.25, ERRCON = 1.89e-4;
    Real errmax, h, htemp, tnew;
    int i, n = _sys.getDim();
    Vector<Real> xerr(n), xscale(n), xtemp(n);

    h = htry;           // Set stepsize to the initial trial value.

    // Scaling used to monitor accuracy.
    for (i = 0; i < n; i++)
        xscale[i] = fabs(_x[i]) + fabs(_dxdt[i] * h) + 1e-30;

    for (;;) {
        _stepCalc.calcStep(_sys, _t, _x, _dxdt, h, xtemp, xerr);

        errmax = 0.0;           // Evaluating accuracy.
        for (int i = 0; i < n; i++)
            errmax = std::max(errmax, fabs(xerr[i] / xscale[i]));
        errmax /= eps;          // Scale relative to required tolerance
        if (errmax <= 1.0)
            break;              // Step succeeded. Compute size of next step.

        htemp = SAFETY * h * pow(errmax, PSHRNK);
        // Truncation error too large, reduce stepsize, but no more than a factor of 10.
        if (h >= Real{ 0 })
            h = std::max(htemp, 0.1 * h);
        else
            h = std::min(htemp, 0.1 * h);

        tnew = _t + h;

        if (tnew == _t) throw("stepsize underflow in rkqs");
    }
    // computing size of the next step
    if (errmax > ERRCON)
        _hNext = SAFETY * h * pow(errmax, PGROW);
    else
        _hNext = 5.0 * h;      // No more than a factor of 5 increase

    _hDone = h;
    _t += h;

    for (i = 0; i < n; i++)
        _x[i] = xtemp[i];
}
```

ODESolver class as master integrator

- Templated on stepper
- Gets ODESolver as input
- Produces ODESolverSolution

```
template<class Stepper> class ODESolver
{
    IODESystem& _sys;
    Stepper _stepper;

    // used as reference by stepper!
    Real _curr_t;
    Vector<Real> _curr_x;
    Vector<Real> _curr_dxdt;

public:
    ODESolver(IODESystem& sys)
        : _sys(sys), _stepper(sys, _curr_t, _curr_x, _curr_dxdt)
    {
        _curr_x.Resize(_sys.getDim());
        _curr_dxdt.Resize(_sys.getDim());
    }

    int getDim() { return _sys.getDim(); }

    // ODE system integrator using given stepper for adaptive stepsize control.
    // Integrates starting values ystart[1..nvar] from t1 to t2 with accuracy eps
    ODESolverSolution integrate(const Vector<Real>& initCond,
                                Real t1, Real t2, Real minSaveInterval,
                                Real eps, Real h1, Real hmin = 0) { ... }
};
```

Integrate function

```
// ODE system integrator using given stepper for adaptive stepsize control.
// Integrates starting values ystart[1..nvar] from t1 to t2 with accuracy eps
ODESystemSolution integrate(const Vector<Real>& initCond,
                           Real t1, Real t2, Real minSaveInterval,
                           Real eps, Real h1, Real hmin = 0)
{
    Real xsav, h;
    int i, stepNum, numSavedSteps=0, sysDim = _sys.getDim();
    int expectedSteps = (int)((t2 - t1) / h1) + 1;
    ODESys
```

SOLVING PENDULUM NUMERICALLY

Starting with our differential equation of second order:

$$\frac{d^2\theta}{dt^2} + \frac{g}{\ell} \sin \theta = 0.$$

Transforming to a system of first-order differential equations

TODO

Which we can easily transcribe to ODESystem class representing pendulum

```
class PendulumODE : public IODESystem
{
    Real _Length;
public:
    PendulumODE(Real length) : _Length(length) {}

    int getDim() const override { return 2; }
    void derivs(const Real x, const MML::Vector<Real>& y, MML::Vector<Real>& dydx) const override
    {
        dydx[0] = y[1];
        dydx[1] = -9.81 / _Length * sin(y[0]);
    }
};
```

Solving pendulum with Euler method

We are starting with the simplest method.

```
// alternative way of defining the system with lambda function
ODESystem pendSys(2, [](Real t, const Vector<Real>& x, Vector<Real>& dxdt)
{
    Real Length = 1.0;
    dxdt[0] = x[1];
    dxdt[1] = -9.81 / Length * sin(x[0]);
};

// setting parameters for our simulation
Real t1 = 0.0, t2 = 10.0;
int expectNumSteps = 1000;           // means our step = 20 / 1000 = 0.01
Real initAngle = Utils::DegToRad(30); // initial angle set to 30 degrees
Vector<Real> initCond{ initAngle, 0.0 };
```

```

// solving and getting solutions
ODESystemFixedStepSolver fixedSolver(pendSys, StepCalculators::EulerStepCalc);
ODESystemSolution sol = fixedSolver.integrate(initCond, t1, t2, expectNumSteps);

Vector<Real> sol_x = sol.getTValues();
Vector<Real> sol_y1 = sol.getXValues(0);
Vector<Real> sol_y2 = sol.getXValues(1);

```

Console output

```

// console visualization
std::cout << "\n\n**** Euler method - fixed stepsize *****\n";
std::vector<ColDesc>      vecNames{ ColDesc("t", 11, 2, 'F'),
                                ColDesc("angle", 15, 8, 'F'),
                                ColDesc("ang.vel.", 15, 8, 'F') };
std::vector<Vector<Real>*> vecVals{ &sol_x, &sol_y1, &sol_y2 };

VerticalVectorPrinter vvp(vecNames, vecVals);

vvp.Print();

```

We'll skip example until next section.

```

// visualizing solutions
PolynomInterpRealFunc    solInterpY1 = sol.getSolutionAsPolyInterp(0, 3);
PolynomInterpRealFunc    solInterpY2 = sol.getSolutionAsPolyInterp(1, 3);

Visualizer::VisualizeRealFunction(solInterpY1, "Pendulum - angle in time",
                                  t1, t2, 200, "pendulum_angle_euler.txt");

Visualizer::VisualizeRealFunction(solInterpY2, "Pendulum - ang.vel. in time",
                                  t1, t2, 200, "pendulum_ang_vel_euler.txt");

```

We can also visualize both variables (there are two ways, with the same result).

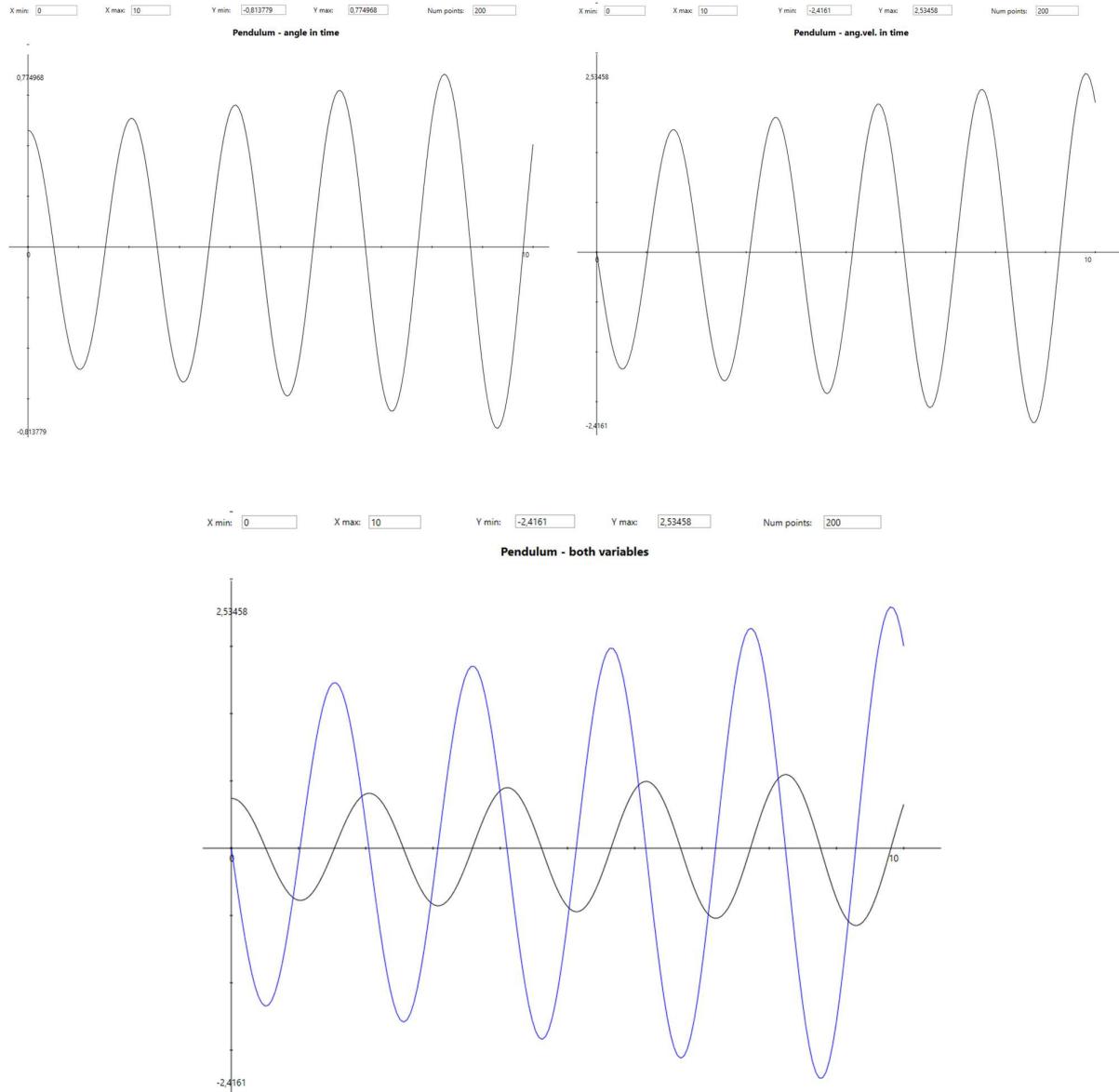
```

// shown together as multi-real function
Visualizer::VisualizeMultiRealFunction({ &solInterpY1, &solInterpY2 },
                                       "Pendulum - both variables", t1, t2, 200,
                                       "pendulum_multi_real_func_euler.txt");

// visualized together as ODE system solution
Visualizer::VisualizeODESysSolAsMultiFunc(sol, "Pendulum - Euler method",
                                           "pendulum_euler.txt");

```

Visualizations



Something is waaay off!?

NEED FOR SYMPLECTING INTEGRATORS THAT CONSERVE PHASE SPACE CONSTRAINTS.

Solving pendulum with our RK4 ODE solvers

Using fixed step-size and adaptive step-size RK solvers to solve it.

```

Real pendulumLen = 1.0;
PendulumODE sys = PendulumODE(pendulumLen);

Real t1 = 0.0, t2 = 10.0;
int expectNumSteps = 100;
Real minSaveInterval = (t2 - t1) / expectNumSteps;
Real initAngle = 0.5;
Vector<Real> initCond{ initAngle, 0.0 };

ODESystemFixedStepSolver fixedSolver(pendSys, StepCalculators::RK4_Basic);
ODESystemSolution solFixed = fixedSolver.integrate(initCond, t1, t2, expectNumSteps);

ODESystemSolver<RK4_CashKarp_Stepper> adaptSolver(sys);
ODESystemSolution solAdapt = adaptSolver.integrate(initCond, t1, t2, minSaveInterval / 1.21, 1e-06, 0.01);

Vector<Real> x_fixed = solFixed.getXValues();
Vector<Real> y1_fixed = solFixed.getYValues(0);
Vector<Real> y2_fixed = solFixed.getYValues(1);

Vector<Real> x_adapt = solAdapt.getXValues();
Vector<Real> y1_adapt = solAdapt.getYValues(0);
Vector<Real> y2_adapt = solAdapt.getYValues(1);

std::cout << "\n\n**** Runge-Kutta 4th order - fixed stepsize ***** Runge-Kutta 4th order - adaptive stepper ****\n";
std::vector<ColDesc> vecNames{ ColDesc("t", 11, 2, 'F'), ColDesc("angle", 15, 8, 'F'), ColDesc("ang.vel.", 15, 8, 'F'),
                           ColDesc("t", 22, 2, 'F'), ColDesc("angle", 12, 8, 'F'), ColDesc("ang.vel.", 12, 8, 'F') };
std::vector<Vector<Real>> vecVals{ &x_fixed, &y1_fixed, &y2_fixed,
                                      &x_adapt, &y1_adapt, &y2_adapt };
VerticalVectorPrinter vvp(vecNames, vecVals);

vvp.Print();

```

Console output

** Runge-Kutta 4th order - fixed step-size ** Runge-Kutta 4th order - adaptive stepper **

t	angle	ang.vel.	t	angle	ang.vel.
0.00	0.50000000	0.00000000	0.00	0.50000000	0.00000000
0.10	0.47665342	-0.46353601	0.13	0.45778475	-0.61776411
0.20	0.40863848	-0.88674198	0.22	0.38831757	-0.97008776
0.30	0.30196570	-1.23045133	0.32	0.28138501	-1.27679705
0.40	0.16638709	-1.45971284	0.42	0.14224787	-1.48447498
0.50	0.01472426	-1.54905478	0.51	0.00100032	-1.54978139
...					
9.20	-0.49774494	0.13629050	9.38	-0.39991174	0.92399290
9.30	-0.46106272	0.59202240	9.47	-0.29786175	1.24013268
9.40	-0.38107371	0.99586669	9.57	-0.16254622	1.46398440
9.50	-0.26491163	1.30947278	9.68	-0.00443368	1.54973588
9.60	-0.12330802	1.50005315	9.83	0.22803362	1.37621501
9.70	0.03023798	1.54600550	9.92	0.33552554	1.14359632
9.80	0.18084654	1.44190607	10.00	0.41786505	0.84481904
9.90	0.31398298	1.19992327			
10.00	0.41709503	0.84673507			

Visualizing solutions graphically

Extracting RealFunction from our discretized ODE solutions.

```
// getting solutions as polynomials
PolynomInterpRealFunc solFixedPolyInterp0 = solFixed.getSolutionAsPolyInterp(0, 3);
PolynomInterpRealFunc solFixedPolyInterp1 = solFixed.getSolutionAsPolyInterp(1, 3);

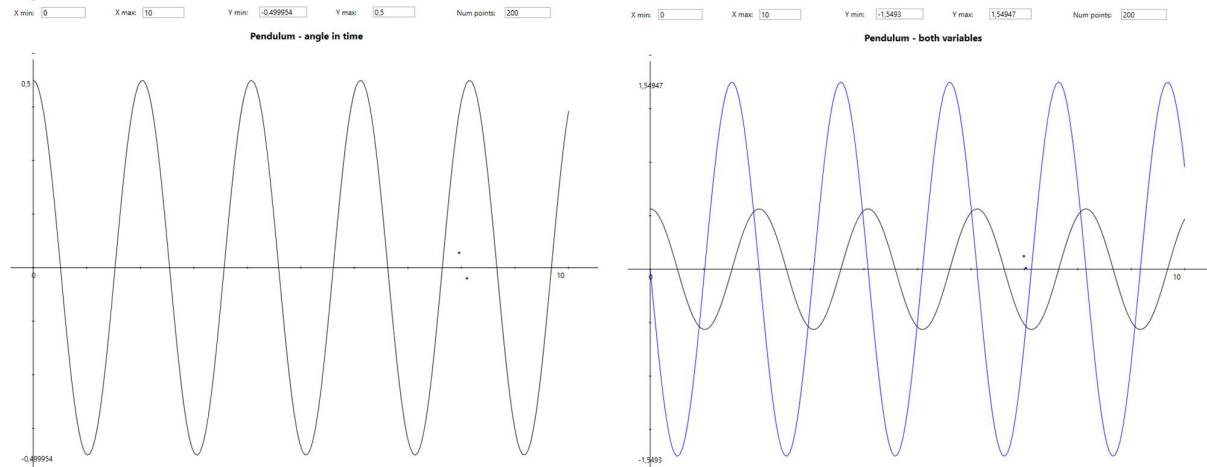
PolynomInterpRealFunc solAdaptPolyInterp0 = solAdapt.getSolutionAsPolyInterp(0, 3);
PolynomInterpRealFunc solAdaptPolyInterp1 = solAdapt.getSolutionAsPolyInterp(1, 3);

SplineInterpRealFunc solSplineInterp0 = solAdapt.getSolutionAsSplineInterp(0);
SplineInterpParametricCurve<2> spline(solAdapt.getYValues());

Visualizer::VisualizeRealFunction(solAdaptPolyInterp0, "Pendulum - angle in time",
                                  0.0, 10.0, 200, "pendulum_angle.txt");

// shown together
Visualizer::VisualizeMultiRealFunction({ &solAdaptPolyInterp0, &solAdaptPolyInterp1 },
                                       "Pendulum - both variables", 0.0, 10.0, 200,
                                       "pendulum_multi_real_func.txt");
```

Vizualizations with vizualizers.



Calculating pendulum period

We are interested in the period of our pendulum, and we can obtain that from solution by analyzing roots of solution functions – checking where they cross abscissa, and looking at distance between neighbor crossing.

```

Real calcFunctionPeriod(const IRealFunction &func, Real t1, Real t2)
{
    int numFoundRoots;
    Vector<Real> root_brack_x1(10), root_brack_x2(10);
    FindRootBrackets(func, t1, t2, 4000, root_brack_x1, root_brack_x2, numFoundRoots);

    Vector<Real> roots(numFoundRoots);
    Vector<Real> rootDiffs(numFoundRoots - 1);
    for (int i = 0; i < numFoundRoots; i++)
    {
        roots[i] = FindRootBisection(func, root_brack_x1[i], root_brack_x2[i], 1e-7);

        if (i > 0)
            rootDiffs[i - 1] = roots[i] - roots[i - 1];
    }

    return Statistics::Avg(rootDiffs);
}

```

We can calculate exact period, based on analytical solution

```

double calculatePendulumPeriod(double length, double initialAngle)
{
    const double g = 9.81;
    double k = std::sin(initialAngle / 2);
    double ellipticIntegral = std::comp_ellint_1(k);

    double period = 4 * std::sqrt(length / g) * ellipticIntegral;

    return period;
}

```

And compare results

```

Real periodLinear = 2.0 * Constants::PI * sqrt(pendulumLen / 9.81);
std::cout << "Pendulum period approx. linear : " << periodLinear << std::endl;

Real simulPeriodFixed = calcFunctionPeriod(solFixedPolyInterp0, t1, t2);
std::cout << "Pendulum period RK4 fixed step : " << 2 * simulPeriodFixed << std::endl;

Real simulPeriodAdapt = calcFunctionPeriod(solAdaptPolyInterp0, t1, t2);
std::cout << "Pendulum period RK4 adapt.step : " << 2 * simulPeriodAdapt << std::endl;

// calculate exact period for pendulum of length L, and given initial angle phi
Real exactPeriod = calculatePendulumPeriod(pendulumLen, initAngle);
std::cout << "Pendulum period analytic exact : " << exactPeriod << std::endl;

```

Pendulum period approx. linear : 2.0060667

Pendulum period RK4 fixed step : 2.0379898

Pendulum period RK4 adapt.step: 2.0378686

Pendulum period analytic exact : 2.0378679

Investigating dependence on initial angle

How does the pendulum period changes, depending on initial angle (ie, how much was pendulum deflected from equilibrium position).

Code

```
Vector<Real> initAnglesDeg{ 1, 2, 5, 10.0, 20.0, 30.0, 40.0, 50.0, 60.0, 70.0, 80.0 };
Vector<Real> initAngles(initAnglesDeg.size());           // convert to radians
for (int i = 0; i < initAngles.size(); i++)
    initAngles[i] = initAnglesDeg[i] * Constants::PI / 180.0;

Vector<Real> periods(initAngles.size());
Real periodLin, periodSimulFixed, periodSimulAdapt, periodExact;

std::cout << "\nAngle      Linear.      Exact      Fix.step.sim Adapt.step.sim" << std::endl;
for (int i = 0; i < initAngles.size(); i++)
{
    initCond[0] = initAngles[i];

    // calculate period from fixed solution
    ODESyste...solF = fixedSolver.integrate(initCond, t1, t2, expectNumSteps);
    PolynomInterpRealFunc solFInterp = solF.getSolutionAsPolyInterp(0, 3);
    periodSimulFixed = calcFunctionPeriod(solFInterp, t1, t2);

    // calculate period from adaptive solution
    ODESyste...solA = adaptSolver.integrate(initCond, t1, t2, minSaveInterval, 1e-06, 0.01);
    PolynomInterpRealFunc solAInterp = solA.getSolutionAsPolyInterp(0, 3);
    periodSimulAdapt = calcFunctionPeriod(solAInterp, t1, t2);

    // analytical formulas
    periodLin = 2.0 * Constants::PI * sqrt(pendulumLen / 9.81);
    periodExact = calculatePendulumPeriod(pendulumLen, initAngles[i]);

    std::cout << std::setw(2) << initAnglesDeg[i] << " deg: " << periodLin << "      "
        << periodExact << "      " << 2 * periodSimulFixed << "      " << 2 * periodSimulAdapt << std::endl;
}
```

TODO – add percentage difference between linear and exact?

Angle	Linear.	Exact	Fix.step.sim	Adapt.step.sim
1 deg:	2.0060667	2.0061049	2.0062607	2.0061015
2 deg:	2.0060667	2.0062195	2.0063751	2.0062195
5 deg:	2.0060667	2.0070219	2.0071766	2.0070184
10 deg:	2.0060667	2.0098926	2.0100438	2.0098799
20 deg:	2.0060667	2.0214513	2.0215905	2.0214573
30 deg:	2.0060667	2.0409899	2.0411092	2.0409933
40 deg:	2.0060667	2.0689379	2.0690328	2.0689287
50 deg:	2.0060667	2.1059346	2.1060029	2.1059113
60 deg:	2.0060667	2.1528747	2.152909	2.1528623
70 deg:	2.0060667	2.2109762	2.2109703	2.2109792
80 deg:	2.0060667	2.2818859	2.2818311	2.2818973

Dependence of number of steps on EPS

Code

```
Vector<Real> acc{ 1e-2, 1e-3, 1e-4, 1e-5, 1e-6, 1e-7, 1e-8 };
Vector<Real> numSteps(acc.size());

std::cout << "\nAccuracy Num steps OK steps Bad steps" << std::endl;
for (int i = 0; i < acc.size(); i++)
{
    ODESolver<RK4_CashKarp_Stepper> adaptSolver(sys);
    ODESolution solAdapt = adaptSolver.integrate(initCond, t1, t2, minSaveInterval, acc[i], 0.01);
    numSteps[i] = solAdapt.getTotalNumSteps();

    std::cout << std::setw(7) << acc[i] << "      " << std::setw(3) << numSteps[i] << "      "
        << std::setw(3) << solAdapt.getNumStepsOK() << "      "
        << std::setw(3) << solAdapt.getNumStepsBad() << std::endl;
}
```

Results

Accuracy	Num steps	OK steps	Bad steps
0.01	17	13	4
0.001	26	17	9
0.0001	40	30	10
1e-05	61	57	4
1e-06	96	91	5
1e-07	157	143	14
1e-08	255	241	14

ADDING AIR RESISTANCE – DUMPED PENDULUM

Basically, it is a dumped oscillating system

```
class DumpedPendulumODE : public IODESystem
{
    Real _length, _dump_coeff;
public:
    DumpedPendulumODE(Real length, Real resistance)
        : _length(length), _dump_coeff(resistance) {}

    int getDim() const override { return 2; }
    void derivs(const Real t, const MML::Vector<Real>& x,
                MML::Vector<Real>& dxdt) const override
    {
        dxdt[0] = x[1];
        dxdt[1] = -9.81 / _length * sin(x[0]) - _dump_coeff * x[1];
    }
};
```

Our standard procedure for solving.

```
DumpedPendulumODE odeSys(1.0, 0.5);

Real t1 = 0.0, t2 = 20.0;
int expectNumSteps = 1000;
Real initAngle = 0.5;
Vector<Real> initCond{ initAngle, 0.0 };

ODESystemFixedStepSolver fixedSolver(odeSys, StepCalculators::RK4_Basic);
ODESystemSolution sol = fixedSolver.integrate(initCond, t1, t2, expectNumSteps);

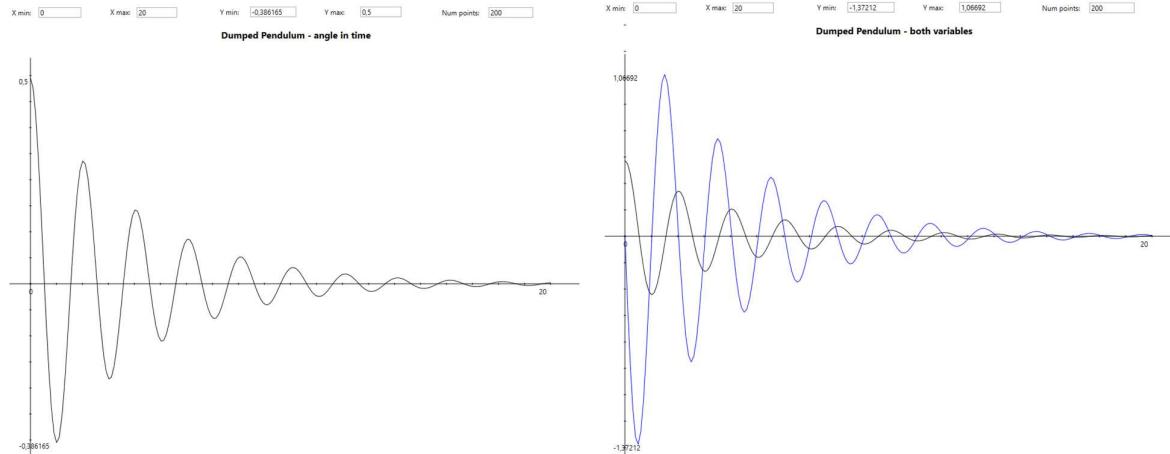
Vector<Real> x_fixed = sol.getTValues();
Vector<Real> y1_fixed = sol.getXValues(0);
Vector<Real> y2_fixed = sol.getXValues(1);
```

And visualizing

```
PolynomInterpRealFunc solInterpY1 = sol.getSolutionAsPolyInterp(0, 3);
PolynomInterpRealFunc solInterpY2 = sol.getSolutionAsPolyInterp(1, 3);

Visualizer::VisualizeRealFunction(solInterpY1, "Dumped Pendulum - angle in time",
                                  t1, t2, 200, "dumped_pendulum_angle.txt");
// shown together
Visualizer::VisualizeMultiRealFunction({ &solInterpY1, &solInterpY2 },
                                         "Dumped Pendulum - both variables",
                                         t1, t2, 200,
                                         "dumped_pendulum_multi_real_func.txt");
```

Visualizations



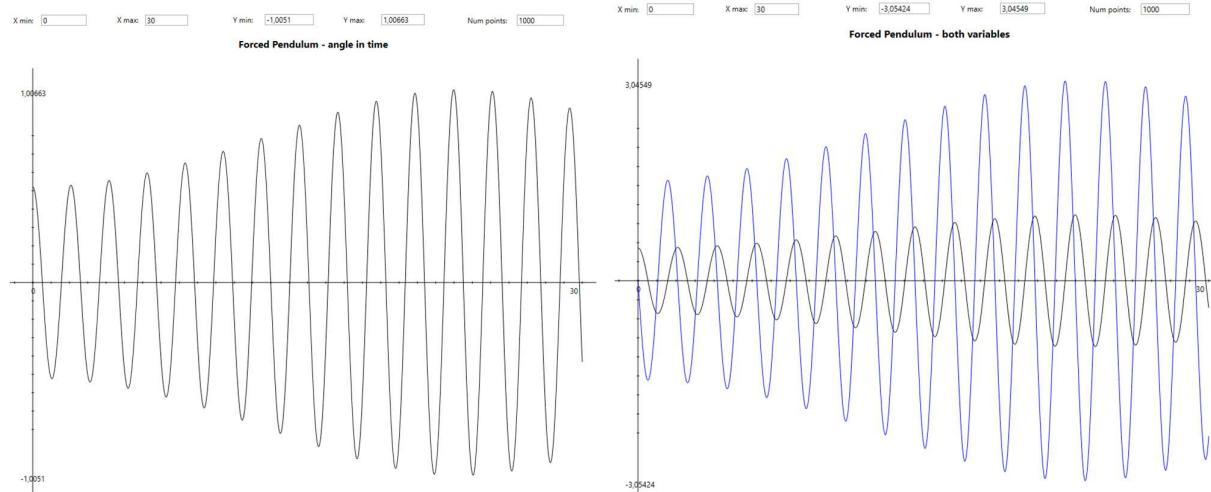
FORCED PENDULUM – RESONANCE

Interesting because of the appearance of resonance.

```
class ForcedPendulumODE : public IODESystem
{
    Real _l, _amp, _period;
public:
    ForcedPendulumODE(Real length, Real forceAmp, Real forcePeriod)
        : _l(length), _amp(forceAmp), _period(forcePeriod) {
    }
    int getDim() const override { return 2; }
    void derivs(const Real t, const MML::Vector<Real>& x,
                MML::Vector<Real>& dxdt) const override
    {
        dxdt[0] = x[1];
        dxdt[1] = -9.81 / _l * sin(x[0]) + _amp * cos(Constants::PI * t / _period);
    }
};
```

Solving

Visualization



6. Spherical and double pendulum – working with Lagrangians

Going all-in with Lagrangian formulation of classical mechanics.

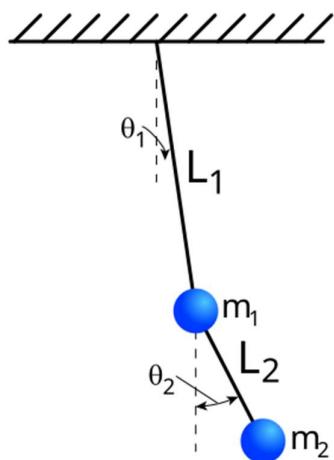
Tasks at hand:

- Introduce basics of Lagrangian formulation of classical mechanics
- Double pendulum as an example
- Spherical pendulum as an example

PHYSICS – LAGRANGIAN FORMULATION IN CLASSICAL MECHANICS

PHYSICS OF DOUBLE PENDULUM

There are various types of double pendulums – compound, ...



Lagrangian for double pendulum:

$$L = \frac{1}{2}m_1(l_1\dot{\theta}_1)^2 + \frac{1}{2}m_2(l_1^2\dot{\theta}_1^2 + l_2^2\dot{\theta}_2^2 + 2l_1l_2\dot{\theta}_1\dot{\theta}_2\cos(\theta_1 - \theta_2)) + m_1gl_1\cos(\theta_1) + m_2g(l_1\cos(\theta_1) + l_2\cos(\theta_2))$$

Solving Euler-Lagrange equations for given Lagrangian gives us two differential equations of motion:

$$(m_1 + m_2)l_1\ddot{\alpha}_1 + m_2l_2\ddot{\alpha}_2 \cos(\alpha_1 - \alpha_2) + m_2l_2\dot{\alpha}_2^2 \sin(\alpha_1 - \alpha_2) + (m_1 + m_2)g \sin \alpha_1 = 0$$

$$l_2\ddot{\alpha}_2 + l_1\ddot{\alpha}_1 \cos(\alpha_1 - \alpha_2) - l_1\dot{\alpha}_1^2 \sin(\alpha_1 - \alpha_2) + g \sin \alpha_2 = 0$$

Using computer algebra package, they can be solved to get expressions for theta1 and theta2

$$\theta_1'' = \frac{-g(2m_1 + m_2)\sin\theta_1 - m_2g\sin(\theta_1 - 2\theta_2) - 2\sin(\theta_1 - \theta_2)m_2(\theta_2'^2 L_2 + \theta_1'^2 L_1 \cos(\theta_1 - \theta_2))}{L_1(2m_1 + m_2 - m_2\cos(2\theta_1 - 2\theta_2))}$$

$$\theta_2'' = \frac{2\sin(\theta_1 - \theta_2)(\theta_1'^2 L_1(m_1 + m_2) + g(m_1 + m_2)\cos\theta_1 + \theta_2'^2 L_2 m_2 \cos(\theta_1 - \theta_2))}{L_2(2m_1 + m_2 - m_2\cos(2\theta_1 - 2\theta_2))}$$

Reducing to set of 4 first-order ODE's we get:

$$\theta_1' = \omega_1$$

$$\theta_2' = \omega_2$$

$$\omega_1' = \frac{-g(2m_1 + m_2)\sin\theta_1 - m_2g\sin(\theta_1 - 2\theta_2) - 2\sin(\theta_1 - \theta_2)m_2(\omega_2^2 L_2 + \omega_1^2 L_1 \cos(\theta_1 - \theta_2))}{L_1(2m_1 + m_2 - m_2\cos(2\theta_1 - 2\theta_2))}$$

$$\omega_2' = \frac{2\sin(\theta_1 - \theta_2)(\omega_1^2 L_1(m_1 + m_2) + g(m_1 + m_2)\cos\theta_1 + \omega_2^2 L_2 m_2 \cos(\theta_1 - \theta_2))}{L_2(2m_1 + m_2 - m_2\cos(2\theta_1 - 2\theta_2))}$$

No analytical solutions are known, so the only thing we can do is try to solve these equations numerically.

NUMERICALLY SOLVING DOUBLE PENDULUM

First, we define a class DoublePendulumODE, that will represent differential equations of motion.

```

class DoublePendulumODE : public IODESystem
{
    Real _m1, _m2;
    Real _l1, _l2;
public:
    DoublePendulumODE(Real m1, Real m2, Real l1, Real l2) : _m1(m1), _m2(m2), _l1(l1), _l2(l2) {}

    int getDim() const override { return 4; }
    void derivs(const Real t, const MML::Vector<Real>& x, MML::Vector<Real>& dxdt) const override
    {
        Real th1 = x[0];
        Real w1 = x[1];
        Real th2 = x[2];
        Real w2 = x[3];

        Real g = 9.81;
        Real divisor = (2 * _m1 + _m2 - _m2 * cos(2*th1 - 2*th2));

        dxdt[0] = w1;
        dxdt[1] = (-g * (2 * _m1 + _m2) * sin(th1) - _m2 * g * sin(th1 - 2 * th2) -
                    2 * sin(th1 - th2) * _m2 * (POW2(w2) * _l2 + POW2(w1) * _l1 * cos(th1 - th2)))
                    / (_l1 * divisor);
        dxdt[2] = w2;
        dxdt[3] = (2 * sin(th1 - th2) * (POW2(w1) * _l1 * (_m1 + _m2) +
                    g * (_m1 + _m2) * cos(th1) +
                    POW2(w2) * _l2 * _m2 * cos(th1 - th2)))
                    / (_l2 * divisor);
    }
};


```

Solving

```

void Demo_DoublePendulum()
{
    Real l1 = 1.0, l2 = 1.0;
    Real m1 = 0.5, m2 = 1.0;
    DoublePendulumODE odeSysDoublePend = DoublePendulumODE(m1, m2, l1, l2);

    Real t1 = 0.0, t2 = 10.0;
    int expectNumSteps = 100;
    Real minSaveInterval = (t2 - t1) / expectNumSteps;
    Real initAngle1 = 0.5;
    Real initAngle2 = 0.1;
    Vector<Real> initCond{ initAngle1, 0.0, initAngle2, 0.0 };

    ODESolver<RK4_CashKarp_Stepper> adaptSolver(odeSysDoublePend);
    ODESolution sol = adaptSolver.integrate(initCond, t1, t2, minSaveInterval, 1e-06, 0.01);
}

```

Printing in console

```

Vector<Real> t_vals      = sol.getXValues();
Vector<Real> theta1_vals = sol.getYValues(0);
Vector<Real> theta2_vals = sol.getYValues(2);

std::cout << "\n\n**** Solving double pendulum ****\n";
std::vector<ColDesc>      vecNames{ ColDesc("t", 11, 2, 'F'),
                                     ColDesc("theta 1", 15, 8, 'F'),
                                     ColDesc("theta 2", 15, 8, 'F'), };
std::vector<Vector<Real>>* vecVals{ &t_vals, &theta1_vals, &theta2_vals };

VerticalVectorPrinter vvp(vecNames, vecVals);
vvp.Print();

```

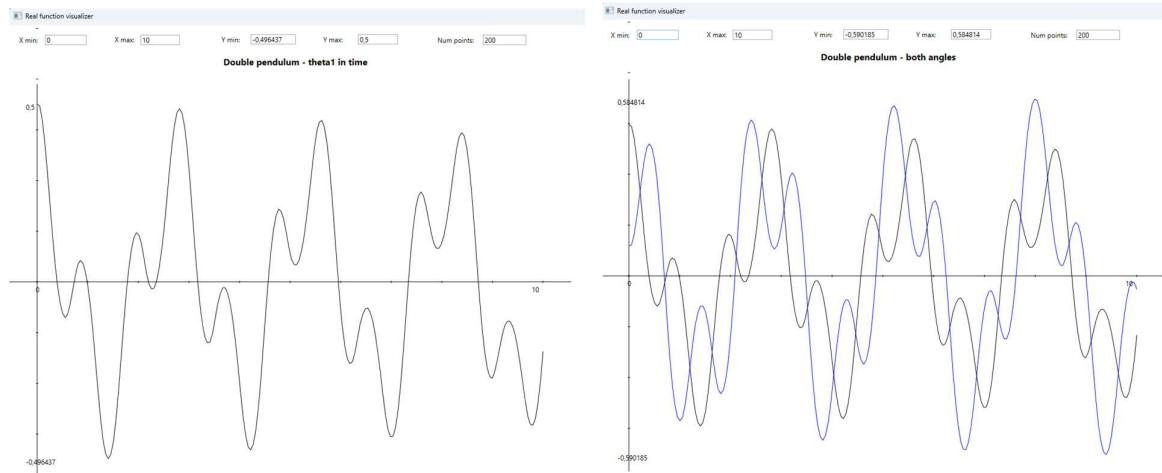
Visualizing graphically

```
// getting solutions as polynomials
PolynomInterpRealFunc solAdaptPolyInterp0 = sol.getSolutionAsPolyInterp(0, 3);
PolynomInterpRealFunc solAdaptPolyInterp1 = sol.getSolutionAsPolyInterp(2, 3);

Visualizer::VisualizeRealFunction(solAdaptPolyInterp0,
    "Double pendulum - theta1 in time",
    0.0, 10.0, 200, "double_pendulum_angle1.txt");

// shown together
Visualizer::VisualizeMultiRealFunction({ &solAdaptPolyInterp0, &solAdaptPolyInterp1 },
    "Double pendulum - both angles", 0.0, 10.0, 200,
    "double_pendulum_multi_real_func.txt");
```

Results



Visualizing phase space of two solutions with slightly different initial conditions.

We have to form a parametric curve in 2D from solutions.

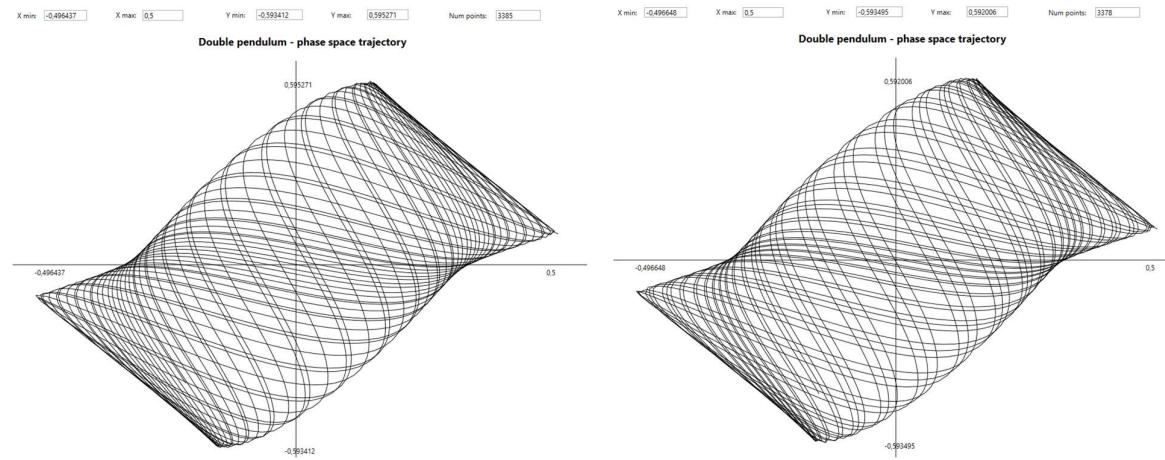
```
// form parametric curve 2d from solution
Matrix<Real> curve_points(t_vals.size(), 2);
for (int i = 0; i < t_vals.size(); i++)
{
    curve_points(i, 0) = theta1_vals[i];
    curve_points(i, 1) = theta2_vals[i];
}

SplineInterpParametricCurve<2> phaseSpaceTrajectory(0.0, 1.0, curve_points);

Visualizer::VisualizeParamCurve2D(phaseSpaceTrajectory, "Double pendulum - phase space trajectory",
    0.0, 1.0, t_vals.size(), "double_pendulum_phase_space.txt");
```

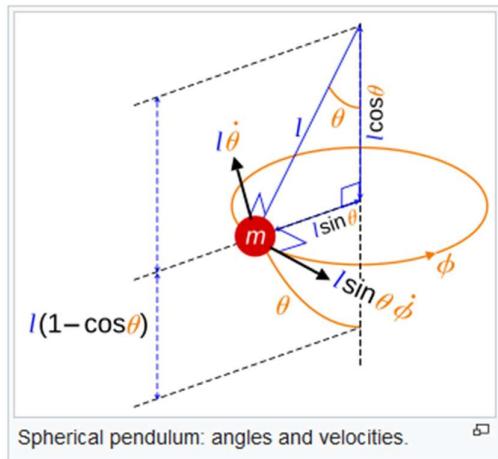
First : initAngle2 = 0.1

Second: initAngle2 = 0.101



PHYSICS OF SPHERICAL PENDULUM

Theoretical introduction mostly taken from Wikipedia (AND MUCH TO DO HERE!)



Hamiltonian formulation.

The Hamiltonian is

$$H = P_\theta \dot{\theta} + P_\phi \dot{\phi} - L$$

where conjugate momenta are

$$P_\theta = \frac{\partial L}{\partial \dot{\theta}} = ml^2 \cdot \dot{\theta}$$

and

$$P_\phi = \frac{\partial L}{\partial \dot{\phi}} = ml^2 \sin^2 \theta \cdot \dot{\phi}.$$

In terms of coordinates and momenta it reads

$$H = \underbrace{\left[\frac{1}{2} ml^2 \dot{\theta}^2 + \frac{1}{2} ml^2 \sin^2 \theta \dot{\phi}^2 \right]}_T + \underbrace{\left[-mgl \cos \theta \right]}_V = \frac{P_\theta^2}{2ml^2} + \frac{P_\phi^2}{2ml^2 \sin^2 \theta} - mgl \cos \theta$$

Where we are aiming for four first order differential equations of motion

$$\begin{aligned}\dot{\theta} &= \frac{P_\theta}{ml^2} \\ \dot{\phi} &= \frac{P_\phi}{ml^2 \sin^2 \theta} \\ \dot{P}_\theta &= \frac{P_\phi^2}{ml^2 \sin^3 \theta} \cos \theta - mgl \sin \theta \\ \dot{P}_\phi &= 0\end{aligned}$$

NUMERICALLY SOLVING SPHERICAL PENDULUM

We can represent this ODE's system as ODESSystem class for our solvers.

```
class SphericalPendulumHamiltonODE : public IODESystem
{
    Real _m, _l;
public:
    SphericalPendulumHamiltonODE() : _l(1.0), _m(1.0) {}
    SphericalPendulumHamiltonODE(Real l) : _l(l), _m(1.0) {}
    SphericalPendulumHamiltonODE(Real m, Real l) : _m(m), _l(l) {}

    int getDim() const override { return 4; }
    void derivs(const Real t, const MML::Vector<Real>& x, MML::Vector<Real>& dxdt) const override
    {
        Real tht = x[0];
        Real phi = x[1];
        Real P_tht = x[2];
        Real P_phi = x[3];

        Real g = 9.81;

        dxdt[0] = P_tht / (_m * POW2(_l));
        dxdt[1] = P_phi / (_m * POW2(_l * sin(tht)));
        dxdt[2] = POW2(P_phi) * cos(tht) / (_m * POW2(_l) * POW3(sin(tht))) - _m * g * _l * sin(tht);
        dxdt[3] = 0.0;
    }
};
```

When solving it, initial conditions are crucial.

```
SphericalPendulumHamiltonODE      odeSysSpherPend = SphericalPendulumHamiltonODE(l);

Real   t1 = 0.0, t2 = 20.0;
int    expectNumSteps = 2000;
Real   minSaveInterval = (t2 - t1) / expectNumSteps;

Real   initAngleTheta = Constants::PI / 2;
Real   initAnglePhi = 0.0;
Vector<Real>  initCond{ initAngleTheta, initAnglePhi, 5.10, -3.55 };
```

Solving it and getting solutions

```
ODESystemSolver<RK5_CashKarp_Stepper> odeSolver(odeSysSpherPend);
ODESystemSolution odeSol = odeSolver.integrate(initCond, t1, t2, minSaveInterval, 1e-07, 0.01);

Vector<Real> t_vals      = odeSol.getTValues();
Vector<Real> theta_vals = odeSol.getXValues(0);
Vector<Real> phi_vals   = odeSol.getXValues(1);
Vector<Real> theta_dot_vals = odeSol.getXValues(2);
Vector<Real> phi_dot_vals = odeSol.getXValues(3);
```

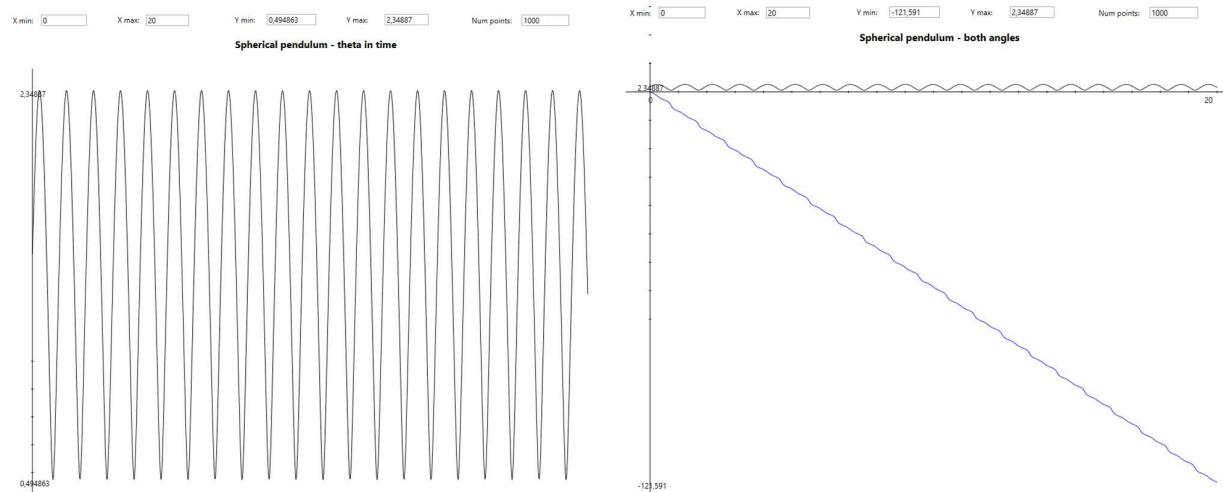
Visualizing solutions

```
// getting solutions as polynomials
PolynomInterpRealFunc  solAdaptPolyInterp0 = odeSol.getSolutionAsPolyInterp(0, 3);
PolynomInterpRealFunc  solAdaptPolyInterp1 = odeSol.getSolutionAsPolyInterp(1, 3);

Visualizer::VisualizeRealFunction(solAdaptPolyInterp0, "Spherical pendulum - theta in time",
                                  t1, t2, 200, "spherical_pendulum_theta.txt");

// shown together
Visualizer::VisualizeMultiRealFunction({ &solAdaptPolyInterp0, &solAdaptPolyInterp1 },
                                       "Spherical pendulum - both angles", { "Theta", "Phi" },
                                       t1, t2, 200,
                                       "spherical_pendulum_multi_real_func.txt");
```

OUPS!!!



There's a surprise!!! TODO – investigate! 😊

Visualization of phase space

```
// projecting pendulum path on x-y, x-z and y-z plane
// first, get values for x, y, z coordinates in vectors
Vector<Real> x_vals(t_vals.size()), y_vals(t_vals.size()), z_vals(t_vals.size());

for (int i = 0; i < t_vals.size(); i++)
{
    x_vals[i] = l * sin(theta_vals[i]) * cos(phi_vals[i]);
    y_vals[i] = l * sin(theta_vals[i]) * sin(phi_vals[i]);
    z_vals[i] = l * (1 - cos(theta_vals[i]));
}

// then form appropriate matrices with relevant data for visualization of parametric curves
Matrix<Real> curve_x_y_points(t_vals.size(), 2), curve_x_z_points(t_vals.size(), 2);
Matrix<Real> curve_y_z_points(t_vals.size(), 2);
Matrix<Real> curve_xyz_points(t_vals.size(), 3);
for (int i = 0; i < t_vals.size(); i++)
{
    curve_xyz_points(i, 0) = 100 * x_vals[i];
    curve_xyz_points(i, 1) = 100 * y_vals[i];
    curve_xyz_points(i, 2) = 100 * z_vals[i];

    curve_x_y_points(i, 0) = x_vals[i];
    curve_x_y_points(i, 1) = y_vals[i];

    curve_x_z_points(i, 0) = x_vals[i];
    curve_x_z_points(i, 1) = z_vals[i];

    curve_y_z_points(i, 0) = y_vals[i];
    curve_y_z_points(i, 1) = z_vals[i];
}
```

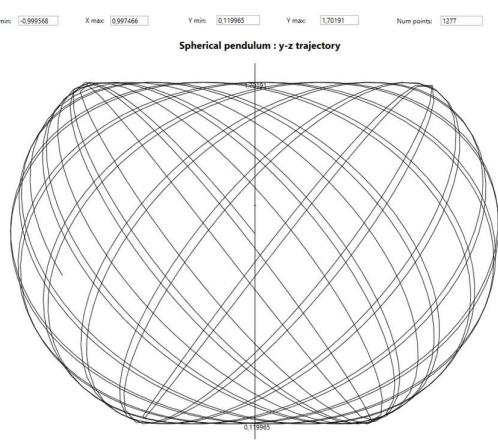
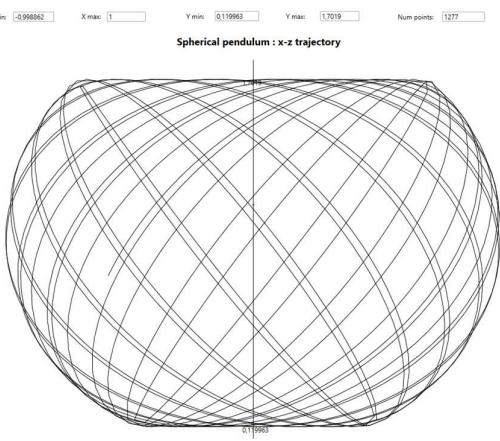
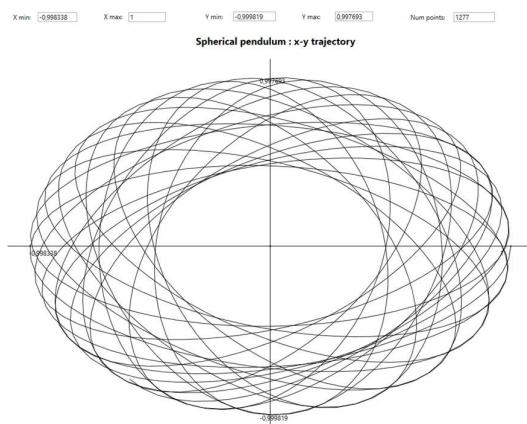
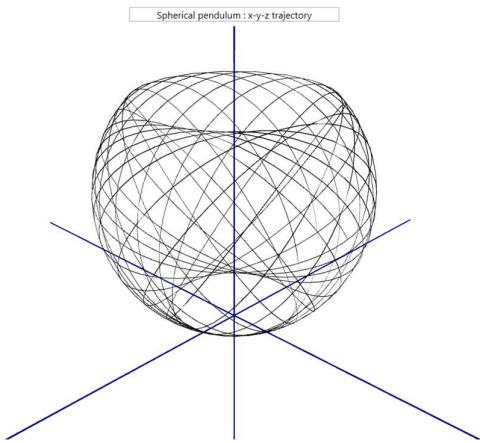
Visualizing

```
SplineInterpParametricCurve<3> xyzTrajectory(0.0, 1.0, curve_xyz_points);
Visualizer::VisualizeParamCurve3D(xyzTrajectory, "Spherical pendulum : x-y-z trajectory",
                                  0.0, 1.0, t_vals.size(), "spherical_pendulum_xyz_trajectory.txt");

SplineInterpParametricCurve<2> xyTrajectory(0.0, 1.0, curve_x_y_points);
Visualizer::VisualizeParamCurve2D(xyTrajectory, "Spherical pendulum : x-y trajectory",
                                  0.0, 1.0, t_vals.size(), "spherical_pendulum_xy_trajectory.txt");

SplineInterpParametricCurve<2> xzTrajectory(0.0, 1.0, curve_x_z_points);
Visualizer::VisualizeParamCurve2D(xzTrajectory, "Spherical pendulum : x-z trajectory",
                                 0.0, 1.0, t_vals.size(), "spherical_pendulum_xz_trajectory.txt");

SplineInterpParametricCurve<2> yzTrajectory(0.0, 1.0, curve_y_z_points);
Visualizer::VisualizeParamCurve2D(yzTrajectory, "Spherical pendulum : y-z trajectory",
                                 0.0, 1.0, t_vals.size(), "spherical_pendulum_yz_trajectory.txt");
```



7. Hitting a ball with a baseball bat

Working it all the way for real situation.

Tasks at hand:

- What happens when we hit a baseball with a baseball bat?
- Adding air resistance
- Adding effect of drag
- Adding effect of spin

From author perspective, it would be more logical to use soccer as an example, but alas, interaction between footballer's leg and soccer ball is, in its determination of initial conditions and simulation of motion, much, much complex problem, so baseball will do.

VACUUM SOLUTION

AIR RESISTANCE

EFFECT OF BASEBALL PROPERTIES ON DRAG

8. Central potential – gravity field

Investigating that all-present force in our lives ... gravity.

Tasks at hand:

- Verify Kepler laws in central potential
- Path integrals for work and potential
- Simulate gravity within Solar system.
- Gravitational slingshot

PHYSICS OF GRAVITATIONAL FIELD

Bazične formule centralnog potencijala, Keplerovi zakoni

Solving two body problem numerically

Verificirati numerički simulacijom two-body problem

Ali, standardni RungeKutta neće biti baš dobar!

Trebati će nam symplectic solvers ... u idućem poglavljju

MATH - FIELD OPERATIONS – GRAD, DIV, CURLS AND ALL THAT JAZZ

Gravity is an excellent example of a simple **field**.

Contour plot of gravity potential as basis for gradient definition

Gradient

Divergence

Curl

Laplacian

IMPLEMENTING FIELD OPERATIONS IN C++

Scalar field operations – gradient and Laplacian

```
namespace ScalarFieldOperations
{
    // ...
    template<int N>
    static VectorN<Real, N> Gradient(const IScalarFunction<N>& scalarField, const VectorN<Real, N>& pos,
                                      const MetricTensorField<N>& metricTensorField) { ... }

    template<int N>
    static Real Divergence(const IVectorFunction<N>& vectorField, const VectorN<Real, N>& pos,
                           const MetricTensorField<N>& metricTensorField) { ... }

    // ...
    template<int N>
    static VectorN<Real, N> GradientCart(const IScalarFunction<N>& scalarField, const VectorN<Real, N>& pos)
    template<int N>
    static VectorN<Real, N> GradientCart(const IScalarFunction<N>& scalarField, const VectorN<Real, N>& pos,
                                         int der_order) { ... }

    static Vec3Sph GradientSpher(const IScalarFunction<3>& scalarField, const Vec3Sph& pos) { ... }
    static Vec3Sph GradientSpher(const IScalarFunction<3>& scalarField, const Vec3Sph& pos,
                                int der_order) { ... }

    static Vec3Cyl GradientCyl(const IScalarFunction<3>& scalarField, const Vec3Cyl& pos) { ... }
    static Vec3Cyl GradientCyl(const IScalarFunction<3>& scalarField, const Vec3Cyl& pos,
                               int der_order) { ... }

    // ...
    template<int N>
    static Real LaplacianCart(const IScalarFunction<N>& scalarField, const VectorN<Real, N>& pos) { ... }
    static Real LaplacianSpher(const IScalarFunction<3>& scalarField, const Vec3Sph& pos) { ... }
    static Real LaplacianCyl(const IScalarFunction<3>& scalarField, const Vec3Cyl& pos) { ... }
};
```

Calculation of a gradient in spherical coordinates

```
static Vec3Sph GradientSpher(const IScalarFunction<3>& scalarField, const Vec3Sph& pos)
{
    Vector3Spherical ret = Derivation::DerivePartialAll<3>(scalarField, pos, nullptr);

    ret[1] = ret[1] / pos[0];
    ret[2] = ret[2] / (pos[0] * sin(pos[1]));

    return ret;
}
```

VectorField operations – divergence & curl

```
namespace VectorFieldOperations
{
    // ...
    template<int N>
    static Real DivCart(const IVectorFunction<N>& vectorField, const VectorN<Real, N>& pos) { ... }
    static Real DivSpher(const IVectorFunction<3>& vectorField, const VectorN<Real, 3>& x) { ... }
    static Real DivCyl(const IVectorFunction<3>& vectorField, const VectorN<Real, 3>& x) { ... }

    // ...
    static Vec3Cart CurlCart(const IVectorFunction<3>& vectorField, const VectorN<Real, 3>& pos) { ... }
    static Vec3Sph CurlSpher(const IVectorFunction<3>& vectorField, const VectorN<Real, 3>& pos) { ... }
    static Vec3Cyl CurlCyl(const IVectorFunction<3>& vectorField, const VectorN<Real, 3>& pos) { ... }
};
```

Calculating divergence in spherical coordinates.

```
static Real DivSpher(const IVectorFunction<3>& vectorField, const VectorN<Real, 3>& x)
{
    VectorN<Real, 3> vals = vectorField(x);

    VectorN<Real, 3> derivs;
    for (int i = 0; i < 3; i++)
        derivs[i] = Derivation::DeriveVecPartial<3>(vectorField, i, i, x, nullptr);

    Real div = 0.0;
    div += 1 / (x[0] * x[0]) * (2 * x[0] * vals[0] + x[0] * x[0] * derivs[0]);
    div += 1 / (x[0] * sin(x[1])) * (cos(x[1]) * vals[1] + sin(x[1]) * derivs[1]);
    div += 1 / (x[0] * sin(x[1])) * derivs[2];

    return div;
}
```

Calculating curl

```
static Vec3Cart CurlCart(const IVectorFunction<3>& vectorField, const VectorN<Real, 3>& pos)
{
    Real dxdy = Derivation::DeriveVecPartial<3>(vectorField, 2, 1, pos, nullptr);
    Real dydz = Derivation::DeriveVecPartial<3>(vectorField, 1, 2, pos, nullptr);

    Real dxz = Derivation::DeriveVecPartial<3>(vectorField, 0, 2, pos, nullptr);
    Real dzdx = Derivation::DeriveVecPartial<3>(vectorField, 2, 0, pos, nullptr);

    Real dydx = Derivation::DeriveVecPartial<3>(vectorField, 1, 0, pos, nullptr);
    Real dxz = Derivation::DeriveVecPartial<3>(vectorField, 0, 1, pos, nullptr);

    Vector3Cartesian curl{ dxdy - dydz, dxz - dzdx, dydx - dxz };

    return curl;
}

static Vec3Sph CurlSpher(const IVectorFunction<3>& vectorField, const VectorN<Real, 3>& pos)
{
    VectorN<Real, 3> vals = vectorField(pos);

    Real dphidtheta = Derivation::DeriveVecPartial<3>(vectorField, 2, 1, pos, nullptr);
    Real dthetadphi = Derivation::DeriveVecPartial<3>(vectorField, 1, 2, pos, nullptr);

    Real drdphi = Derivation::DeriveVecPartial<3>(vectorField, 0, 2, pos, nullptr);
    Real dphidr = Derivation::DeriveVecPartial<3>(vectorField, 2, 0, pos, nullptr);

    Real dthetadr = Derivation::DeriveVecPartial<3>(vectorField, 1, 0, pos, nullptr);
    Real drdtheta = Derivation::DeriveVecPartial<3>(vectorField, 0, 1, pos, nullptr);

    Vector3Spherical ret;
    const Real& r = pos[0];
    const Real& theta = pos[1];
    const Real& phi = pos[2];

    ret[0] = 1 / (r * sin(theta)) * (cos(theta) * vals[2] + sin(theta) * dphidtheta - dthetadphi);
    ret[1] = 1 / r * (1 / sin(theta) * drdphi - vals[2] - r * dphidr);
    ret[2] = 1 / r * (vals[1] + r * dthetadr - drdtheta);

    return ret;
}
```

Testing implementation on gravity field

For gravitational field we can calculate analytically values for gradient, divergence and curl, and it is a perfect situation to verify how good are our numerically calculated values.

MATH - PATH INTEGRATION

Calculating work between two points along different curves connecting them, and verify with potential calculation

IMPLEMENTING PATH INTEGRATION IN C++

```
class PathIntegration
{
    template<int N>
    class HelperCurveLen { ... };

    template<int N>
    class HelperCurveMass { ... };

    template<int N>
    class HelperLineIntegralScalarFunc { ... };

    template<int N>
    class HelperLineIntegralVectorFunc { ... };

public:
    template<int N>
    static Real ParametricCurveLength(const IParametricCurve<N>& curve, const Real a, const Real b) { ... }

    template<int N>
    static Real ParametricCurveMass(const IParametricCurve<N>& curve, const IRealFunction &density,
                                   const Real a, const Real b) { ... }

    static Real LineIntegral(const IScalarFunction<3>& scalarField, const IParametricCurve<3>& curve,
                           const Real a, const Real b, const Real eps = Defaults::WorkIntegralPrecision) { ... }

    static Real LineIntegral(const IVectorFunction<3>& vectorField, const IParametricCurve<3>& curve,
                           const Real a, const Real b, const Real eps = Defaults::LineIntegralPrecision) { ... }
};
```

SIMULATING GRAVITY IN SOLAR SYSTEM

Setup of all planet orbits and simulation of satellite motion through it (Voyager?).

Building SolarSystemSimulator

Simulating Voyager path through Solar system

GRAVITATIONAL SLINGSHOT – HOW IT WORKS?

9. Simulating gravity properly in N-body problem

Deep dive with gravity simulation.

Tasks at hand:

- Numerically simulate N-body problem
- Symplectic integrators

NEED FOR SYMPLECTIC ODE SOLVERS

In time independent Hamiltonian system, the energy and the phase space volume are conserved and special integration methods have to be applied in order to ensure these conservation laws.

SIMULATING N-BODY GRAVITATIONAL PROBLEM IN C++

Modeling gravity mass and N-body configuration, with initial conditions.

```
class GravityMass
{
public:
    Real _mass;
    Vector3Cartesian _position;
    Vector3Cartesian _velocity;

    GravityMass(const Real& mass, const Vector3Cartesian& position)
        : _mass(mass), _position(position) {}
    GravityMass(const Real& mass, const Vector3Cartesian& position, const Vector3Cartesian& velocity)
        : _mass(mass), _position(position), _velocity(velocity) {}
};

class NBodyGravityConfig
{
    std::vector<GravityMass> _masses;
public:
    int NumBodies() const { return (int)_masses.size(); }

    void AddBody(Real mass, Vector3Cartesian position, Vector3Cartesian velocity)
    {
        _masses.push_back(GravityMass(mass, position, velocity));
    }

    Real Mass(int i) const { return _masses[i]._mass; }
    Vector3Cartesian Position(int i) const { return _masses[i]._position; }
    Vector3Cartesian Velocity(int i) const { return _masses[i]._velocity; }

    void SetPosition(int i, Vector3Cartesian pos) { _masses[i]._position = pos; }
    void SetVelocity(int i, Vector3Cartesian vel) { _masses[i]._velocity = vel; }
};
```

Simple Euler solver

```
class NBodyMotionSolverEuler
{
protected:
    NBodyGravityConfig _config;

public:
    NBodyMotionSolverEuler(NBodyGravityConfig inConfig) : _config(inConfig) { }

    void simulateOneStep(const Real dt)
    {
        std::vector<Vector3Cartesian> force(_config.NumBodies(), Vector3Cartesian(0.0, 0.0, 0.0));

        for (int i = 0; i < _config.NumBodies(); i++) {
            // calculate force on body i
            for (int j = 0; j < _config.NumBodies(); j++) {
                if (i != j) {
                    Real gravityConstant = 30;
                    Vec3Cart radialVec = _config.Position(i) - _config.Position(j);
                    force[i] = force[i] - gravityConstant * _config.Mass(i) * _config.Mass(j) / POW3(radialVec.NormL2()) * radialVec;
                }
            }
        }
        // advancing velocities and positions, using the most simple Euler method of first order
        for (int i = 0; i < _config.NumBodies(); i++) {
            _config.SetVelocity(i, _config.Velocity(i) + force[i] * dt / _config.Mass(i));
            _config.SetPosition(i, _config.Position(i) + _config.Velocity(i) * dt);
        }
    }

    std::vector<std::vector<VectorN<Real, 3>>> simulate(const Real dt, const int steps)
    {
        std::vector<std::vector<VectorN<Real, 3>>> trajectories(_config.NumBodies());

        // saving initial positions
        for (int i = 0; i < _config.NumBodies(); i++)
            trajectories[i].push_back(_config.Position(i));

        for (int i = 0; i < steps; i++) {
            simulateOneStep(dt);

            for (int i = 0; i < _config.NumBodies(); i++)
                trajectories[i].push_back(_config.Position(i));
        }
        return trajectories;
    }
};
```

Main program, with setup, simulation and visualization

```
NBodyGravityConfig config;
config.AddBody(10000, Vector3Cartesian{ 0.0, 0.0, 0.0 }, Vector3Cartesian{ 0.0, 0.0, 0.0 });
config.AddBody(20, Vector3Cartesian{ -110.0, -50.0, 10.0 }, Vector3Cartesian{ 0.0, 50, 0.0 });
config.AddBody(10, Vector3Cartesian{ 130.0, 50.0, 70.0 }, Vector3Cartesian{ 0.0, -50, 0 });
config.AddBody(20, Vector3Cartesian{ -20.0, 100.0, -110.0 }, Vector3Cartesian{ 50, 0.0, 0.0 });
config.AddBody(10, Vector3Cartesian{ 70.0, -110.0, 70.0 }, Vector3Cartesian{ -50, 50, 50.0 });

NBodyMotionSolverEuler solver(config);

const Real dt      = 0.01;
const int  steps   = 2000;

auto res = solver.simulate(dt, steps);

for (int i = 0; i < config.NumBodies(); i++)
{
    Serializer::SaveAsParamCurve<3>(res[i], "PARAMETRIC_CURVE_CARTESIAN_3D", "Body" + std::to_string(i+1),
                                         0.0, dt * steps, steps + 1,
                                         MML_PATH_ResultFiles + "body" + std::to_string(i) + ".txt");
}

Visualizer::VisualizeMultiParamCurve3D({"body0.txt", "body1.txt", "body2.txt", "body3.txt", "body4.txt"});
```

Resulting trajectories



Defining ODE system for N-body problem

```

class NBodySystemODE : public IODESystem
{
    NBodyGravityConfig _config;
    const Real G = 6.67430e-11;

public:
    NBodySystemODE(NBodyGravityConfig inConfig) : _config(inConfig) { }

    int getDim() const { return 3 * _config.NumBodies(); }
    void derivs(const Real t, const Vector<Real>& x, Vector<Real>& dxdt) const
    {
        // filling in dxdt vector with N * 6 derivations of our variables (x, y, z, vx, vy, vz)
        for (int i = 0; i < _config.NumBodies(); i++)
        {
            // calculating force on body i
            Vector3Cartesian force(0, 0, 0);
            for (int j = 0; j < _config.NumBodies(); j++)
            {
                if (i != j)      // checking for self-force
                {
                    Vector3Cartesian vec_dist(dxdt[6 * j] - dxdt[6 * i],
                                                dxdt[6 * j + 2] - dxdt[6 * i + 2],
                                                dxdt[6 * j + 4] - dxdt[6 * i + 4]);

                    force = force - G * _config.Mass(i) * _config.Mass(j) / POW3(vec_dist.NormL2()) * vec_dist;
                }
            }

            // x coord
            dxdt[6 * i]      = x[6 * i + 1];
            dxdt[6 * i + 1] = 1 / _config.Mass(i) * force.X();
            // y coord
            dxdt[6 * i + 2] = x[6 * i + 3];
            dxdt[6 * i + 3] = 1 / _config.Mass(i) * force.Y();
            // z coord
            dxdt[6 * i + 4] = x[6 * i + 5];
            dxdt[6 * i + 5] = 1 / _config.Mass(i) * force.Z();
        }
    }
};

```

Main program

TODO

LONG TERM SIMULATION!

Using symplectic integrators!

Runge-Kutta-Nystroem solvers

Visualizing fields

10. Coordinate transformations

Contravariant and covariant vectors ... and all that jazz.

Tasks at hand:

- Modelling general coordinate transformations in C++
- Implement various transformations
- Oblique systems and difference between contravariant and covariant vectors

TRANSFORMATION OF COORDINATES

Different characterizations/types of coordinate systems

- Homogenous / non-homogenous
- Orthogonal / oblique
- Linear / curvilinear

General transformation of coordinates:

$$\begin{cases} \bar{x}^1 = f^1(x^1, \dots, x^n), \\ \dots, \\ \bar{x}^n = f^n(x^1, \dots, x^n), \end{cases}$$

Or in short notation,

$$\bar{x}^j = f^j(x^k) \quad (j = 1, \dots, n).$$

It is assumed we also have an inverse transformation.

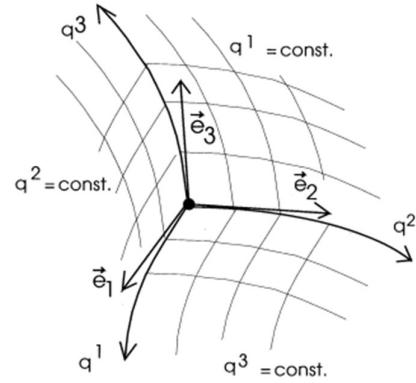
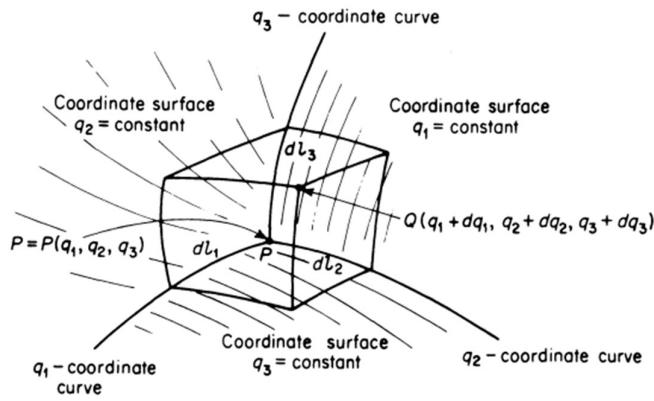
Polar coordinates in 2D

Rotations in 2D

Orthogonal transformations

Curvilinear

Visualization of general curvilinear coordinate system



Spherical

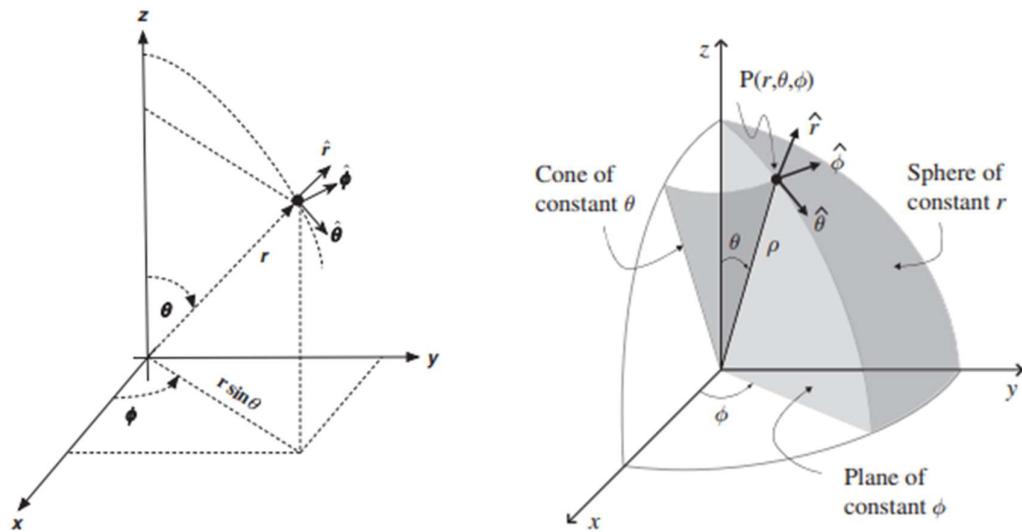


Figure 23. Spherical system coordinates

Transformation formulas. First, from a set of Cartesian coordinates (x, y, z) to spherical (r, θ, ϕ)

$$r = \sqrt{x^2 + y^2 + z^2}$$

$$\theta = \cos^{-1}(z/r)$$

$$\phi = \tan^{-1}(y/x),$$

And the inverse transformation, from spherical to Cartesian.

$$x = r \sin \theta \cos \phi$$

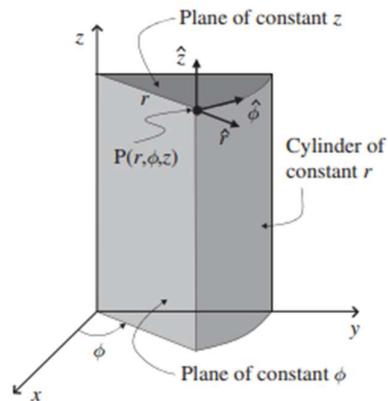
$$y = r \sin \theta \sin \phi$$

$$z = r \cos \theta.$$

TODO - Mathematical and physical convention in ordering coordinates.

Cylindrical

Cylindrical coordinate system is extension of 2D polar coordinate system to 3 dimensions, by simply including z as third coordinate.



Transformation from Cartesian to cylindrical.

$$r = \sqrt{x^2 + y^2}$$

$$\theta = \arctan\left(\frac{y}{x}\right)$$

$$z = z$$

And inverse.

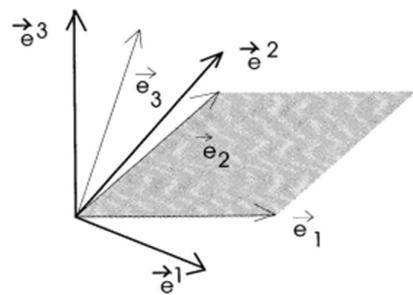
$$x = r \cos(\phi)$$

$$y = r \sin(\phi)$$

$$z = z.$$

Oblique Cartesian coordinate system

Dual basis



Constructing reciprocal (dual) basis in 3D.

TRANSFORMING VECTORS

Covariant and contravariant vectors

Vector3Spherical

```

class Vector3Spherical : public VectorN<Real, 3>
{
public:
    Real R() const { return _val[0]; }
    Real& R() { return _val[0]; }
    Real Theta() const { return _val[1]; }
    Real& Theta() { return _val[1]; }
    Real Phi() const { return _val[2]; }
    Real& Phi() { return _val[2]; }

    Vector3Spherical() : VectorN<Real, 3>{ 0.0, 0.0, 0.0 } {}
    Vector3Spherical(const VectorN<Real, 3>& b) : VectorN<Real, 3>{ b[0], b[1], b[2] } {}
    Vector3Spherical(Real r, Real theta, Real phi) : VectorN<Real, 3>{ r, theta, phi } {}
    Vector3Spherical(std::initializer_list<Real> list) : VectorN<Real, 3>(list) {}

    Vector3Spherical GetAsUnitVectorAtPos(const Vector3Spherical& pos) const { ... }

    std::ostream& PrintDeg(std::ostream& stream, int width, int precision) const { ... }
};


```

Vector3Cylindrical

```

class Vector3Cylindrical : public VectorN<Real, 3>
{
public:
    Real R() const { return _val[0]; }
    Real& R() { return _val[0]; }
    Real Phi() const { return _val[1]; }
    Real& Phi() { return _val[1]; }
    Real Z() const { return _val[2]; }
    Real& Z() { return _val[2]; }

    Vector3Cylindrical() : VectorN<Real, 3>{ 0.0, 0.0, 0.0 } {}
    Vector3Cylindrical(const VectorN<Real, 3>& b) : VectorN<Real, 3>{ b[0], b[1], b[2] } {}
    Vector3Cylindrical(Real r, Real phi, Real z) : VectorN<Real, 3>{ r, phi, z } {}
    Vector3Cylindrical(std::initializer_list<Real> list) : VectorN<Real, 3>(list) {}

    Vector3Cylindrical GetAsUnitVectorAtPos(const Vector3Cylindrical& pos) const { ... }

};


```

IMPLEMENTING COORDINATE TRANSFORMATIONS IN C++

We define two basic interfaces.

Why inheriting from IVectorFunction? Because every coordinate transformation is actually defined through vector function – function that takes vector of original coordinates, and returns vector of transformed coordinates.

```

template<typename VectorFrom, typename VectorTo, int N>
class ICoordTransf : public IVectorFunction<N>
{
public:
    virtual      VectorTo      transf(const VectorFrom& in) const = 0;
    virtual const IScalarFunction<N>& coordTransfFunc(int i) const = 0;

    virtual ~ICoordTransf() {}
};

```

For transformations that have an inverse, we specialize original interface, requiring

```

template<typename VectorFrom, typename VectorTo, int N>
class ICoordTransfWithInverse : public virtual ICoordTransf<VectorFrom, VectorTo, N>
{
public:
    virtual      VectorFrom      transfInverse(const VectorTo& in) const = 0;
    virtual const IScalarFunction<N>& inverseCoordTransfFunc(int i) const = 0;

    virtual ~ICoordTransfWithInverse() {}
};

```

We need explicit form of each transformation function, so we can do mathematical operations on those functions.

Then we create two abstract classes, that will be base classes for all our coordinate transformations.

```

template<typename VectorFrom, typename VectorTo, int N>
class CoordTransf : public virtual ICoordTransf<VectorFrom, VectorTo, N>
{
public:
    // inherited from IVectorFunction
    VectorN<Real, N> operator()(const VectorN<Real, N>& x) const
    {
        VectorN<Real, N> ret;
        for (int i = 0; i < N; i++)
            ret[i] = this->coordTransfFunc(i)(x);
        return ret;
    }

    virtual VectorTo  getBasisVec(int ind, const VectorFrom& pos) { ... }
    virtual VectorFrom getInverseBasisVec(int ind, const VectorFrom& pos) { ... }

    MatrixNM<Real, N, N> jacobian(const VectorN<Real, N>& pos) { ... }

    VectorTo  transfVecContravariant(const VectorFrom& vec, const VectorFrom& pos) { ... }
    VectorFrom transfInverseVecCovariant(const VectorTo& vec, const VectorFrom& pos) { ... }
};

```

```

template<typename VectorFrom, typename VectorTo, int N>
class CoordTransfWithInverse : public virtual CoordTransf<VectorFrom, VectorTo, N>,
                                public virtual ICoordTransfWithInverse<VectorFrom, VectorTo, N>
{
public:
    virtual VectorFrom getContravarBasisVec(int ind, const VectorTo& pos) { ... }
    virtual VectorTo    getInverseContravarBasisVec(int ind, const VectorTo& pos) { ... }

    VectorTo    transfVecContravariant(const VectorFrom& vec, const VectorTo& pos) { ... }
    VectorFrom  transfInverseVecContravariant(const VectorTo& vec, const VectorTo& pos) { ... }

    Tensor2<N> transfTensor2(const Tensor2<N>& tensor, const VectorFrom& pos) { ... }
    Tensor3<N> transfTensor3(const Tensor3<N>& tensor, const VectorFrom& pos) { ... }
    Tensor4<N> transfTensor4(const Tensor4<N>& tensor, const VectorFrom& pos) { ... }
    Tensor5<N> transfTensor5(const Tensor5<N>& tensor, const VectorFrom& pos) { ... }
};


```

Essence of this classes, and main reason for their existence, is in the set of 'transf' functions, where we implement general transformation rules for vectors (and tensors), that will be available in all classes that inherit from this abstract classes.

```

VectorTo    transfVecContravariant(const VectorFrom& vec, const VectorFrom& pos)
{
    VectorFrom ret;
    for (int i = 0; i < N; i++) {
        ret[i] = 0;
        for (int j = 0; j < N; j++)
            ret[i] += Derivation::NDer4Partial(this->coordTransfFunc(i), j, pos) * vec[j];
    }
    return ret;
}

```

And also, transformation of covariant vector:

```

VectorTo    transfVecCovariant(const VectorFrom& vec, const VectorTo& pos)
{
    VectorTo ret;
    for (int i = 0; i < N; i++)
    {
        ret[i] = 0;
        for (int j = 0; j < N; j++)
            ret[i] += Derivation::NDer4Partial(this->inverseCoordTransfFunc(j), i, pos) * vec[j];
    }
    return ret;
}

```

Finally, example implementation for concrete spherical to cartesian transformation.

```

class CoordTransfSphericalToCartesian : public CoordTransfWithInverse<Vector3Spherical, Vector3Cartesian, 3>
{
private:
    // q[0] = r      - radial distance
    // q[1] = theta - inclination
    // q[2] = phi   - azimuthal angle
    static Real x(const VectorN<Real, 3>& q) { return q[0] * sin(q[1]) * cos(q[2]); }
    static Real y(const VectorN<Real, 3>& q) { return q[0] * sin(q[1]) * sin(q[2]); }
    static Real z(const VectorN<Real, 3>& q) { return q[0] * cos(q[1]); }

    // ...
    static Real r(const VectorN<Real, 3>& q) { return sqrt(q[0]*q[0] + q[1]*q[1] + q[2]*q[2]); }
    static Real theta(const VectorN<Real, 3>& q) { return acos(q[2] / sqrt(q[0]*q[0] + q[1]*q[1] + q[2]*q[2])); }
    static Real phi(const VectorN<Real, 3>& q) { return atan2(q[1], q[0]); }

    inline static ScalarFunction<3> _func[3] = { ScalarFunction<3>{x},
                                                ScalarFunction<3>{y},
                                                ScalarFunction<3>{z} };
};

inline static ScalarFunction<3> _funcInverse[3] = { ScalarFunction<3>{r},
                                                ScalarFunction<3>{theta},
                                                ScalarFunction<3>{phi} };
};

public:
    Vector3Cartesian    transf(const Vector3Spherical& q) const { return Vector3Cartesian{ x(q), y(q), z(q) }; }
    Vector3Spherical    transfInverse(const Vector3Cartesian& q) const { return Vector3Spherical{ r(q), theta(q), phi(q) }; }

    const IScalarFunction<3>& coordTransfFunc(int i) const { return _func[i]; }
    const IScalarFunction<3>& inverseCoordTransfFunc(int i) const { return _funcInverse[i]; }
}

```

Example of a RotationXAxis transformation, that unlike spherical transformation, depends on a parameter (angle of rotation).

```

class CoordTransfCart3DRotationXAxis :
    public CoordTransfWithInverse<Vector3Cartesian, Vector3Cartesian, 3>
{
private:
    Real    _angle;
    MatrixNM<Real, 3, 3> _transf;
    MatrixNM<Real, 3, 3> _inverse;

    const ScalarFunctionFromStdFunc<3> _f1, _f2, _f3;
    const ScalarFunctionFromStdFunc<3> _fInverse1, _fInverse2, _fInverse3;
}

```

For coordinate transformations that depend on parameters (and so can't be made completely static), fun begins with the constructor:

```

CoordTransfCart3DRotationXAxis(Real inAngle) : _angle(inAngle),
    _f1(std::function<Real(const VectorN<Real, 3>&)>
        { std::bind(&CoordTransfCart3DRotationXAxis::func1, this, std::placeholders::_1) }
    ),
    _f2(std::function<Real(const VectorN<Real, 3>&)>
        { std::bind(&CoordTransfCart3DRotationXAxis::func2, this, std::placeholders::_1) }
    ),
    _f3(std::function<Real(const VectorN<Real, 3>&)>
        { std::bind(&CoordTransfCart3DRotationXAxis::func3, this, std::placeholders::_1) }
    ),
    _fInverse1(std::function<Real(const VectorN<Real, 3>&)>
        { std::bind(&CoordTransfCart3DRotationXAxis::funcInverse1, this, std::placeholders::_1) }
    ),
    _fInverse2(std::function<Real(const VectorN<Real, 3>&)>
        { std::bind(&CoordTransfCart3DRotationXAxis::funcInverse2, this, std::placeholders::_1) }
    ),
    _fInverse3(std::function<Real(const VectorN<Real, 3>&)>
        { std::bind(&CoordTransfCart3DRotationXAxis::funcInverse3, this, std::placeholders::_1) }
    )
{
    _transf[0][0] = 1.0;
    _transf[1][1] = cos(_angle);
    _transf[1][2] = -sin(_angle);
    _transf[2][1] = sin(_angle);
    _transf[2][2] = cos(_angle);

    _inverse[0][0] = 1.0;
    _inverse[1][1] = cos(_angle);
    _inverse[1][2] = sin(_angle);
    _inverse[2][1] = -sin(_angle);
    _inverse[2][2] = cos(_angle);
}

```

TODO – finish example

11. All is not well, if you are in a non-inertial frame!

Wouldn't you know, there are some "fictitious" forces in classical mechanics?

Tasks at hand:

- Investigating centripetal forces on a simple 2D carousel

PHYSICS OF ROTATING SYSTEMS

SIMPLE CAROUSEL AND CENTRIFUGAL FORCE

Carousel with radius of 20 meters, throwing darts

3 pikada, ako baci točno u centar (u njeovom coord sustavu), gdje će strelica završiti

INTRODUCING REFERENTIAL FRAME

Carousel on carousel 😊

Shooting method za ODE's?

12. Projectile/rocket launch

Launching projectiles ... what could be more fun.

Tasks at hand:

- A projectile is fired from the center of Ban Jelačić Square in Zagreb ($45^{\circ}48'47.4''N$ $15^{\circ}58'38.3''E$) at an angle of 45 degrees, in eastward direction. Ignoring air resistance, what is position of the projectile after one hour, for following values of the initial velocity (in m/s): 200, 1.000, 10.000, 15.000?
- What if we include air resistance?
- How can we simulate rocket motors (ie. the “projectile” doesn’t get all its speed at the start)

ARTILLERY GRENADE – 200 M/S

Coriolis force enters the scene!

BALLISTIC ROCKET – 1000 M/S

LOW ORBIT SATELLITE – 10000 M/S

HITTING THE MOON AND BEYOND – 15000 M/S

We will revisit this problem for special relativity velocities

13. Rigid body

Point-like mechanical particles are great ... but there is more to mechanics than that.

Task at hand:

- Simple body pushed with some force in space without gravity, how it moves and rotates?
- Spinning top without gravity
- Tensors
- Eigenvalues

introducing tensors and their transformations

PHYSICS OF RIGID BODY

Moment of inertia

Eigenvalues

Euler equations

IMPLEMENTING TENSORS IN C++

Basic interface for rank 2 tensor (similar defined up to rank 5).

```
template<int N>
class ITensor2
{
public:
    virtual int NumContravar() const = 0;
    virtual int NumCovar() const = 0;

    virtual Real operator()(int i, int j) const = 0;
    virtual Real& operator()(int i, int j) = 0;
};
```

Concrete implementation

```
template <int N>
class Tensor2 : public ITensor2<N>
{
    MatrixNM<Real, N, N> _coeff;
public:
    int _numContravar = 0;
    int _numCovar = 0;
    bool _isContravar[2];

    Tensor2(int nCovar, int nContraVar){ ... }
    Tensor2(int nCovar, int nContraVar, std::initializer_list<Real> values){ ... }

    int NumContravar() const { return _numContravar; }
    int NumCovar() const { return _numCovar; }

    bool IsContravar(int i) const { return _isContravar[i]; }
    bool IsCovar(int i) const { return !_isContravar[i]; }

    Real operator()(int i, int j) const override { return _coeff[i][j]; }
    Real& operator()(int i, int j) override { return _coeff[i][j]; }

    Tensor2 operator+(const Tensor2& other) const{ ... }
    Tensor2 operator-(const Tensor2& other) const{ ... }
    Tensor2 operator*(Real scalar) const{ ... }
    Tensor2 operator/(Real scalar) const{ ... }

    friend Tensor2 operator*(Real scalar, const Tensor2& b){ ... }

    Real Contract() const{ ... }
    Real operator()(const VectorN<Real, N>& v1, const VectorN<Real, N>& v2) const{ ... }

    void Print(std::ostream& stream, int width, int precision) const{ ... }
    friend std::ostream& operator<<(std::ostream& stream, const Tensor2& a){ ... }
};
```

TENSOR TRANSFORMATIONS

Transformation of rank 2 tensor.

Member of CoordTransfWithInverse abstract class, and available for every inherited coordinate transformation class.

```
Tensor2<N> transTensor2(const Tensor2<N>& tensor, const VectorFrom& pos)
{
    Tensor2<N> ret(tensor.NumContravar(), tensor.NumCovar());

    for (int i = 0; i < N; i++)
        for (int j = 0; j < N; j++)
    {
        ret(i, j) = 0;
        for (int k = 0; k < N; k++)
            for (int l = 0; l < N; l++)
        {
            double coef1, coef2;
            if (tensor._isContravar[0])
                coef1 = Derivation::NDer1Partial(this->coordTransfFunc(i), k, pos);
            else
                coef1 = Derivation::NDer1Partial(this->inverseCoordTransfFunc(k), i, pos);

            if (tensor._isContravar[1])
                coef2 = Derivation::NDer1Partial(this->coordTransfFunc(j), l, pos);
            else
                coef2 = Derivation::NDer1Partial(this->inverseCoordTransfFunc(l), j, pos);

            ret(i, j) += coef1 * coef2 * tensor(k, l);
        }
    }

    return ret;
}
```

CALCULATING MOMENT OF INERTIA

Calculating moment of inertia for a set of discrete masses

Necessary models:

```
struct DiscreteMass {
    Vector3Cartesian _position;
    double _mass;

    DiscreteMass(const Vector3Cartesian &position, const double& mass)
        : _position(position), _mass(mass) { }

};

struct DiscreteMassesConfig {
    std::vector<DiscreteMass> _masses;

    DiscreteMassesConfig(const std::vector<DiscreteMass>& masses)
        : _masses(masses) { }

};
```

Calculator

```
class DiscreteMassMomentOfInertiaTensorCalculator
{
    DiscreteMassesConfig _massesConfig;
public:
    DiscreteMassMomentOfInertiaTensorCalculator(const DiscreteMassesConfig& massesConfig)
        : _massesConfig(massesConfig) {}

    Tensor2<3> calculate()
    {
        Tensor2<3> tensor(2,0); // can be (0,2) or (1,1) as well (it is a Cartesian tensor)
        for (const auto& mass : _massesConfig._masses)
        {
            Vector3Cartesian pos = mass._position;
            tensor(0,0) += mass._mass * (pos.Y() * pos.Z() + pos.Z() * pos.Z());
            tensor(1,1) += mass._mass * (pos.X() * pos.X() + pos.Z() * pos.Z());
            tensor(2,2) += mass._mass * (pos.X() * pos.X() + pos.Y() * pos.Y());

            tensor(0,1) -= mass._mass * pos.X() * pos.Y();
            tensor(0,2) -= mass._mass * pos.X() * pos.Z();
            tensor(1,2) -= mass._mass * pos.Y() * pos.Z();

            tensor(1,0) = tensor(0,1);
            tensor(2,0) = tensor(0,2);
            tensor(2,1) = tensor(1,2);
        }
        return tensor;
    }
};
```

Calculating moment of inertia for continuous mass

CALCULATING EIGENVALUES

SIMULATING RIGID BODY

14. Rotations and quaternions

Orientation, orientation, orientation ... and transformation.

Tasks at hand:

- Rotations
- Quaternions

REPRESENTING ROTATIONS

QUATERNIONS

15. Motion in spacetime – Lorentz transformations

When your speed approaches speed of light, strange things tend to happen.

Tasks at hand:

- Basics of special relativity and Lorentz transformations
- Introduce Vector4Lorentz and LorentzTransformation classes

PHYSICS OF SPECIAL RELATIVITY

Vector4Lorentz

Adding time as coordinate for specifying vectors in four-dimensional spacetime.

Per almost universal custom, time coordinate is first one, with convenient index 0.

```
class Vector4Lorentz : public VectorN<Real, 4>
{
public:
    Real T() const { return _val[0]; }
    Real& T() { return _val[0]; }
    Real X() const { return _val[1]; }
    Real& X() { return _val[1]; }
    Real Y() const { return _val[2]; }
    Real& Y() { return _val[2]; }
    Real Z() const { return _val[3]; }
    Real& Z() { return _val[3]; }

    Vector4Lorentz() : VectorN<Real, 4>{ 0.0, 0.0, 0.0, 0.0 } {}
    Vector4Lorentz(std::initializer_list<Real> list) : VectorN<Real, 4>(list) {}
};
```

LorentzTransformation

TODO – general Lorentz transformation, for a boost in any direction

```

class CoordTransfLorentzXAxis : public CoordTransfWithInverse<Vector4Lorentz, Vector4Lorentz, 4>
{
private:
    Real _velocity;           // expressed in units of c (speed of light)
    MatrixNM<Real, 4, 4> _transf;
    MatrixNM<Real, 4, 4> _inverse;

    const ScalarFunctionFromStdFunc<4> _f1, _f2, _f3, _f4;
    const ScalarFunctionFromStdFunc<4> _fInv1, _fInv2, _fInv3, _fInv4;

```

Monstruous constructor, setting everything up for of transformation function

```

CoordTransfLorentzXAxis(Real inVelocity) : _velocity(inVelocity),
{
    _f1(std::function<Real(const VectorN<Real, 4>&)> { std::bind(&CoordTransfLorentzXAxis::func1, this, std::placeholders::_1) });
    _f2(std::function<Real(const VectorN<Real, 4>&)> { std::bind(&CoordTransfLorentzXAxis::func2, this, std::placeholders::_1) });
    _f3(std::function<Real(const VectorN<Real, 4>&)> { std::bind(&CoordTransfLorentzXAxis::func3, this, std::placeholders::_1) });
    _f4(std::function<Real(const VectorN<Real, 4>&)> { std::bind(&CoordTransfLorentzXAxis::func4, this, std::placeholders::_1) });
    _fInv1(std::function<Real(const VectorN<Real, 4>&)> { std::bind(&CoordTransfLorentzXAxis::funcInverse1, this, std::placeholders::_1) });
    _fInv2(std::function<Real(const VectorN<Real, 4>&)> { std::bind(&CoordTransfLorentzXAxis::funcInverse2, this, std::placeholders::_1) });
    _fInv3(std::function<Real(const VectorN<Real, 4>&)> { std::bind(&CoordTransfLorentzXAxis::funcInverse3, this, std::placeholders::_1) });
    _fInv4(std::function<Real(const VectorN<Real, 4>&)> { std::bind(&CoordTransfLorentzXAxis::funcInverse4, this, std::placeholders::_1) });

    double gamma = 1.0 / sqrt(1.0 - _velocity * _velocity);
    double beta = _velocity;

    _transf[0][0] = gamma;
    _transf[0][1] = -beta * gamma;
    _transf[1][0] = -beta * gamma;
    _transf[1][1] = gamma;
    _transf[2][2] = 1.0;
    _transf[3][3] = 1.0;

    _inverse[0][0] = gamma;
    _inverse[0][1] = -beta * gamma;
    _inverse[1][0] = -beta * gamma;
    _inverse[1][1] = gamma;
    _inverse[2][2] = 1.0;
    _inverse[3][3] = 1.0;
}

```

MATH - INTRODUCING METRIC TENSOR

Implementing metric tensors in C++

Interface for rank two tensor field in N dimensions.

```

template<int N>
class ITensorField2 : public IFunction<Tensor2<N>, const VectorN<Real, N>& >
{
    int _numContravar;
    int _numCovar;
public:
    ITensorField2(int numContra, int numCo) : _numContravar(numContra), _numCovar(numCo) { }

    int getNumContravar() const { return _numContravar; }
    int getNumCovar() const { return _numCovar; }

    // concrete implementations need to provide this
    virtual Real Component(int i, int j, const VectorN<Real, N>& pos) const = 0;

    virtual ~ITensorField2() {}

};


```

Abstract class representing general metric tensor field, defined throughout the whole space.

```

template<int N>
class MetricTensorField : public ITensorField2<N>
{
public:
    MetricTensorField() : ITensorField2<N>(2, 0) { }
    MetricTensorField(int numContra, int numCo) : ITensorField2<N>(numContra, numCo) { }

    // implementing operator() required by IFunction interface
    Tensor2<N> operator()(const VectorN<Real, N>& pos) const
    {
        Tensor2<N> ret(this->getNumContravar(), this->getNumCovar());

        for (int i = 0; i < N; i++)
            for (int j = 0; j < N; j++)
                ret(i, j) = this->Component(i, j, pos);

        return ret;
    }

    Real GetChristoffelSymbolFirstKind(int i, int j, int k, const VectorN<Real, N>& pos) const
    Real GetChristoffelSymbolSecondKind(int i, int j, int k, const VectorN<Real, N>& pos) const

    VectorN<Real, N> CovariantDerivativeContravar(const IVectorFunction<N>& func, int j,
                                                    const VectorN<Real, N>& pos) const { ... }
    Real CovariantDerivativeContravarComp(const IVectorFunction<N>& func, int i, int j,
                                           const VectorN<Real, N>& pos) const { ... }

    VectorN<Real, N> CovariantDerivativeCovar(const IVectorFunction<N>& func, int j,
                                                const VectorN<Real, N>& pos) const { ... }
    Real CovariantDerivativeCovarComp(const IVectorFunction<N>& func, int i, int j,
                                       const VectorN<Real, N>& pos) const { ... }

};


```

Simplest example is metric tensor for Cartesian space in three dimensions.

```

class MetricTensorCartesian3D : public MetricTensorField<3>
{
public:
    MetricTensorCartesian3D() : MetricTensorField<3>(2, 0) { }

    Real Component(int i, int j, const VectorN<Real, 3>& pos) const
    {
        if (i == j)
            return 1.0;
        else
            return 0.0;
    }
};

```

Metric tensor for spherical coordinates comes in two variants.

Covariant

```

class MetricTensorSpherical : public MetricTensorField<3>
{
public:
    MetricTensorSpherical() : MetricTensorField<3>(0, 2) { }

    virtual Real Component(int i, int j, const VectorN<Real, 3>& pos) const override
    {
        if (i == 0 && j == 0)
            return 1.0;
        else if (i == 1 && j == 1)
            return POW2(pos[0]);
        else if (i == 2 && j == 2)
            return pos[0] * pos[0] * sin(pos[1]) * sin(pos[1]);
        else
            return 0.0;
    }
};

```

And contravariant (which is just the inverse of covariant version).

```

class MetricTensorSphericalContravar : public MetricTensorField<3>
{
public:
    MetricTensorSphericalContravar() : MetricTensorField<3>(2, 0) { }

    virtual Real Component(int i, int j, const VectorN<Real, 3>& pos) const
    {
        if (i == 0 && j == 0)
            return 1.0;
        else if (i == 1 && j == 1)
            return 1 / (pos[0] * pos[0]);
        else if (i == 2 && j == 2)
            return 1 / (pos[0] * pos[0] * sin(pos[1]) * sin(pos[1]));
        else
            return 0.0;
    }
};

```

Finally, we come to metric tensor for spacetime, which we will call MetricTensorMinkowski:

```

class MetricTensorMinkowski : public MetricTensorField<4>
{
public:
    MetricTensorMinkowski() : MetricTensorField<4>(2, 0) {}

    virtual Real Component(int i, int j, const VectorN<Real, 4>& pos) const override
    {
        if (i == 0 && j == 0)
            return -1.0;
        else if (i == 1 && j == 1)
            return 1.0;
        else if (i == 2 && j == 2)
            return 1.0;
        else if (i == 3 && j == 3)
            return 1.0;
        else
            return 0.0;
    }
};

```

SOLVED EXAMPLES

Projectile launch with relativistic speed

Continuing our example from Chapter 12, what is position if we launch it with speeds: 0.1c, 0.3c, 0.5c, 0.8c, 0.9c, 0.95c?

Earth gravity and Coriolis force are not relevant here, and the only important thing is where that projectile will appear (!) to be, to Earth observer at the location where it was fired from.

Passenger on train dropping ball

Moving on a train with 0.8c, passenger drops a ball to the floor. At what time it hits the floor for passenger, and stationary observer

Spherical ball passing by observer with relativistic speed

Spherical ball, 1 meter in diameter, is travelling with speed 0.9c along a line that at its closest is 100 meters from observer.

Observer has an extremely fast camera with a tracker that ensures camera is pointed exactly at the centre of the sphere at all times.

16. Special relativity – resolving twin-paradox

Where we investigate the most famous “paradox” of them all.

Task at hand:

- Simulate numerically twin paradox
- Simple case with linear trajectory from A to B
- Realistic case with acceleration and a real trajectory to destination

PHYSICS OF PROPER TIME

NUMERICAL SIMULATION

17. Static electric fields

Starting our investigations in electromagnetism.

Task at hand:

- Calculate electric fields for different charge configurations.
- Investigate numerically Gauss and Stokes law, both in integral and differential form.

PHYSICS – COULOMB LAW

Jednostavno numeričko izračunavanje potencijala za analitički poznata rješenja i usporedba

SIMULATING DISTRIBUTION OF CHARGE ON A SOLID BODY

What is distribution of charge on different solid bodies?

Sfera

Cilindar

Kvadar

Something with “pointy” end

ELECTRIC FIELD OF A ROD WITH FINITE LENGTH

In previous section we calculated distribution of charge

Which means we can now calculate electric field throughout space

But actually, we want field lines visualized

Projection in plane

POTENTIAL AND WORK IN ELECTRIC FIELD

CONDUCTORS AND DIELECTRICS

18. Static magnetic fields

Looking at static magnetic fields.

Task at hand:

- Calculate magnetic fields for different current configurations.

PHYSICS - BIOT-SAVART LAW

Magnetic field of a simple loop with passing current

19. Dynamic EM fields

What happens when charges and currents are not static?

Task at hand:

- Investigate dynamic electromagnetic fields.
- Introduce electro-magnetic tensor
- EM field of a moving charge

PHYSICS – MAXWELL'S EQUATIONS

INTRODUCING EM TENSOR

```
Tensor2<4> GetEMTensorContravariant(Vector3Cartesian E_field, Vector3Cartesian B_field)
{
    double c = 1.0;

    Tensor2<4> EM_tensor(2, 0);

    EM_tensor(0, 0) = 0.0;
    EM_tensor(0, 1) = -E_field.X() / c;
    EM_tensor(0, 2) = -E_field.Y() / c;
    EM_tensor(0, 3) = -E_field.Z() / c;

    EM_tensor(1, 0) = E_field.X() / c;
    EM_tensor(1, 1) = 0.0;
    EM_tensor(1, 2) = -B_field.Z();
    EM_tensor(1, 3) = B_field.Y();

    EM_tensor(2, 0) = E_field.Y() / c;
    EM_tensor(2, 1) = B_field.Z();
    EM_tensor(2, 2) = 0.0;
    EM_tensor(2, 3) = -B_field.X();

    EM_tensor(3, 0) = E_field.Z() / c;
    EM_tensor(3, 1) = -B_field.Y();
    EM_tensor(3, 2) = B_field.X();
    EM_tensor(3, 3) = 0.0;

    return EM_tensor;
}
```

LIENARD-WIECHERT POTENTIAL OF MOVING CHARGE

Basic calculation

```
// Given t and r in lab frame of the observer, calculate Lienard-Wiechert potentials
// for charge moving along x-axis with given velocity
Real calcLienardWiechertScalarPotential(Vector3Cartesian r_at_point, Real t, Vector3Cartesian rs_charge_pos,
                                         Real q, Real charge_velocity)
{
    double c = 3e8;
    Vec3Cart charge_v(charge_velocity, 0, 0);

    // calculate retarded time
    Real r = (r_at_point - rs_charge_pos).NormL2();
    Real tr = t - (r_at_point - rs_charge_pos).NormL2() / c;

    // calculate retarded position
    Vec3Cart r_ret_charge_pos = r_at_point - charge_v * (t - tr);

    Real beta = charge_v.NormL2() / c;
    Vec3Cart ns = (r_at_point - r_ret_charge_pos) / (r_at_point - r_ret_charge_pos).NormL2();

    Real scalar_potential = q / ((r_at_point - r_ret_charge_pos).NormL2() * (1 - beta * ScalarProduct(ns, charge_v) / c));
    return scalar_potential;
}
```

TODO;

Parametrizacija moving naboja, što mu je t?

Imamo grid postavljenih mjeritelja el. Polja, koje s brzinom c vraćaju signale nazad do observera

Ispaljuje se naboј brzinom 0.8 c u t = 0, za observera

Simulacija takva da je u prvih 10 dT, kod observera polja nema, a na 10d dT dođe prvi signal od najbližjeg mjeritelja točki ispaljivanja

SIMPLE ANTENNA?

Varying current through antenna and resulting electric field

20. Differential geometry of curves and surfaces

Diving into some differential geometry with curves and surfaces.

Task at hand:

- Implement numerical calculations of curves and surfaces differential geometry properties.
- Frenet-Serret formulas, moving trihedron
- Connection with velocity and acceleration

CURVES

Mathematics of curves

Most of the formulas are for “arc-length parametrized” curves ... and those are mostly NOT what occurs in practice

TODO – give both set of formulas with intro

Modeling curves in C++

Starting from interface IParametricCurve

```
// abstract class, providing basic curve formulas in 2D
class ICurveCartesian2D : public IParametricCurve<2>
{
public:
    Vec2Cart getTangent(Real t)
    {
        return Derivation::DeriveCurve<2>(*this, t, nullptr);
    }
    Vec2Cart getTangentUnit(Real t)
    {
        return getTangent(t).GetAsUnitVector();
    }
    Vec2Cart getNormal(Real t)
    {
        return Derivation::DeriveCurveSec<2>(*this, t, nullptr);
    }
    Vec2Cart getNormalUnit(Real t)
    {
        return getNormal(t).GetAsUnitVector();
    }
};
```

Set of defined 2D (planar) curves

```
class Circle2DCurve : public ICurveCartesian2D
{
    Real _radius;
    Pnt2Cart _center;
public:
    Circle2DCurve() : _radius(1), _center(0, 0) {}
    Circle2DCurve(Real radius) : _radius(radius), _center(0,0) {}
    Circle2DCurve(Real radius, const Pnt2Cart& center) : _radius(radius), _center(center) {}

    Real getMinT() const { return 0.0; }
    Real getMaxT() const { return 2 * Constants::PI; }

    VectorN<Real, 2> operator()(Real t) const {
        return MML::VectorN<Real, 2>{_center.X() + _radius * cos(t), _center.Y() + _radius * sin(t)};
    }
};

class LogSpiralCurve { ... };

class LemniscateCurve { ... };

class DeltoidCurve { ... };

class AstroidCurve { ... };

class EpitrochoidCurve { ... };

class ArchimedeanSpiralCurve { ... };
```

Going to 3D, we again have an abstract class

```
// abstract class, providing basic curve formulas in 3D
class ICurveCartesian3D : public IParametricCurve<3>
{
public:
    Vec3Cart getTangent(Real t) const
    {
        return Derivation::DeriveCurve<3>(*this, t, nullptr);
    }
    Vec3Cart getTangentUnit(Real t) const
    {
        return getTangent(t).GetAsUnitVector();
    }
    Vec3Cart getNormal(Real t) const
    {
        return Derivation::DeriveCurveSec<3>(*this, t, nullptr);
    }
    Vec3Cart getNormalUnit(Real t) const
    {
        return getNormal(t).GetAsUnitVector();
    }
    Vec3Cart getBinormal(Real t) const
    {
        Vec3Cart tangent = getTangentUnit(t);
        Vec3Cart normal = getNormalUnit(t);

        return VectorProduct(tangent, normal);
    }

    Vec3Cart getCurvatureVector(Real t) const { ... }
    Real getCurvature(Real t) const { ... }
    Real getTorsion(Real t) const { ... }
};
```

And a set of predefined 3D curves

```
class LineCurve { ... };

class Circle3DXY { ... };

class Circle3DXZ { ... };

class Circle3DYZ { ... };

class HelixCurve : public ICurveCartesian3D
{
    Real _radius, _b;
public:
    HelixCurve() : _radius(1.0), _b(1.0) {}
    HelixCurve(Real radius, Real b) : _radius(radius), _b(b) {}

    Real getMinT() const { return Constants::NegativeInf; }
    Real getMaxT() const { return Constants::PositiveInf; }

    VectorN<Real, 3> operator()(Real t) const {
        return MML::VectorN<Real, 3>{_radius * cos(t), _radius * sin(t), _b * t};
    }

    Real getCurvature(Real t) const { return _radius / (POW2(_radius) + POW2(_b)); }
    Real getTorsion(Real t) const { return _b / (POW2(_radius) + POW2(_b)); }
};

class TwistedCubicCurve { ... };

class ToroidalSpiralCurve { ... };
```

Also, a concrete class, useful if you have a function pointer, or curve is simple enough to be defined with lambda.

```
// concrete class, that can be initialized with function pointers or lambdas
class CurveCartesian3D : public ICurveCartesian3D
{
    Real _minT;
    Real _maxT;
    VectorN<Real, 3>(*_func)(Real);
public:
    CurveCartesian3D(VectorN<Real, 3>(*inFunc)(Real)) { ... }
    CurveCartesian3D(Real minT, Real maxT, VectorN<Real, 3>(*inFunc)(Real)) { ... }

    Real getMinT() const { return _minT; }
    Real getMaxT() const { return _maxT; }

    virtual VectorN<Real, 3> operator()(Real x) const { return _func(x); }
};
```

SURFACES

Mathematics of surfaces

Modeling surfaces in C++

LOOKING TO MANIFOLDS

Sphere as a manifold

Can we calculate some geodesics?

21. General relativity

Going to the final frontier.

Task at hand:

- Schwarzschild geometry of black hole. How does crossing the event horizon looks from perspective of observer and traveler.
- How it is different for Kerr metric

EINSTEIN'S EQUATION

STATIC BLACK HOLE - SCHWARZSCHILD'S METRIC

ROTATING BLACK HOLE - KERR METRIC