# ChatGPT for Programming Numerical Methods

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ChatGPT (OpenAI): https://chat.openai.com/chat

## Abstract

ChatGPT is a large language model recently released by the OpenAI company. In this technical report, we explore for the first time the capability of ChatGPT for programming numerical algorithms. Specifically, we examine the capability of GhatGPT for generating codes for numerical algorithms in different programming languages, for debugging and improving written codes by users, for completing missed parts of numerical codes, rewriting available codes in other programming languages, and for parallelizing serial codes. Additionally, we assess if ChatGPT can recognize if given codes are written by humans or machines. To reach this goal, we consider a variety of mathematical problems such as the Poisson equation, the diffusion equation, the incompressible Navier-Stokes equations, compressible inviscid flow, eigenvalue problems, solving linear systems of equations, storing sparse matrices, etc. Furthermore, we exemplify scientific machine learning such as physics-informed neural networks and convolutional neural networks with applications to computational physics. Through these examples, we investigate the successes, failures, and challenges of ChatGPT. Examples of failures are producing singular matrices, operations on arrays with incompatible sizes, programming interruption for relatively long codes, etc. Our outcomes suggest that ChatGPT can successfully program numerical algorithms in different programming languages, but certain limitations and challenges exist that require further improvement of this machine learning model.

**Keywords:** ChatGPT; Numerical algorithms; Scientific simulations; Programming languages; Automation of programming; Natural language processing

# Contents

# 1  Introduction

Numerical algorithms play a critical role in scientific simulations and computational modeling. These algorithms are usually developed and implemented by human programmers using programming languages such as C, C++, Python, MATLAB, etc. Nevertheless, implementing and programming sophisticated numerical algorithms could be potentially challenging tasks.

ChatGPT has been released and introduced by OpenAI in November 2022. The primary goal of designing ChatGPT is to generate natural language text for a wide range of applications (e.g., see Refs. [40, 7]). Now as researchers in the area of computational physics and mathematics, if we think about "codes" as a specific type of text, some questions that come to mind are if ChatGPT can successfully accomplish the task of programming numerical algorithms and if the automation of programming numerical methods can be fully handled by a trained language model such as ChatGPT. ChatGPT bas been examined for its capacity to develop software [49, 2] and automatically fix bugs in codes [41]. Additionally, the categorization of failures by ChatGPT has been reported in Ref. [4]. These research papers [41, 4, 49] studied the ChatGPT performance for coding and programming from a general software engineering point of view. Nevertheless, we carry out the performance of ChatGPT specifically for programming numerical methods in the current report.

In this technical report, we investigate for the first time the capability of ChatGPT for programming numerical algorithms in different programming languages. Particularly, we test the ability of this artificial intelligence model by considering various scientific problems such as the two-dimensional Poisson equation, the two-dimensional diffusion equation, the incompressible Navier-Stokes equations in two dimensions, compressible inviscid flow in one dimension, finding the maximum eigenvalue of matrices, solving linear systems of equations, storing sparse matrices, etc. We also provide examples of scientific machine learning such as convolutional neural networks for supervised learning and physics-informed neural networks for weakly supervised learning in computational mechanics. We analyze the capacity of GhatGPT to debug and enhance user-written codes, complete missing numerical code segments, rewrite existing codes in different programming languages, and parallelize serial codes. Furthermore, we test ChatGPT's ability to determine if given codes were created by humans or machines. Our goal is to explore the successes, failures, and challenges of ChatGPT through these test cases.

The results of our exploration provide insight into the capability of ChatGPT for programming numerical algorithms and the potential of such models for automating the programming of complex scientific simulations. Moreover, this technical report can contribute to the development of new tools and techniques for programming numerical algorithms by the means of natural language processing.

# 2  Programming numerical algorithms by ChatGPT

## 2.1  A simple numerical method

We start with a simple and basic numerical algorithm. There are various methods for finding the roots of a function. Among them, the secant method [30] is an iterative numerical method used to find the root of a function $f(x)$ by approximating the derivative of the function with a finite difference method. The mathematical formulation of the secant method is expressed as

$$x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})}, \tag{1}$$

where $x_k$ and $x_{k-1}$ are the last two approximations to the root. $x_{k+1}$ is the new approximation to the root. $f(x_k)$ and $f(x_{k-1})$ are the function values at $x_k$ and $x_{k-1}$, respectively. We ask ChatGPT to write a Python code for the secant method. The gray boxes below show the input prompt and output from ChatGPT.

> A  Write a Python code for root finding using the secant method.

Sure! Here is a Python code for root finding using the secant method:

```python
def secant_method(f, x0, x1, tol=1e-6, max_iter=100):
    """
    Implements the secant method to find a root of a function f.

    Args:
    f: callable function of one variable
    x0: initial guess for the root
    x1: second initial guess for the root
    tol: tolerance for convergence (default=1e-6)
    max_iter: maximum number of iterations (default=100)

    Returns:
    x: estimate of the root
    """
    i = 0
    while i < max_iter:
        x = x1 - ((f(x1)*(x1 - x0)) / (f(x1) - f(x0)))
        if abs(x - x1) < tol:
            return x
        x0 = x1
        x1 = x
        i += 1
    raise ValueError("Secant method failed to converge.")
```

Here is an example of how to use this function to find a root of a function:

```python
import math

# Define the function to find the root of
def f(x):
    return math.cos(x) - x**3

# Call the secant_method function with initial guesses x0=0.5 and x1=1.0
root = secant_method(f, 0.5, 1.0)

print("Root found:", root)
print("f(root) =", f(root))
```

This will output:

```
Root found: 0.865474030893062
f(root) = 3.552713678800501e-15
```

Note that the secant method is not guaranteed to converge, so it's important to check for convergence and to set a maximum number of iterations to avoid an infinite loop. In this implementation, if the method fails to converge within the maximum number of iterations, a '**ValueError**' is raised.

As can be seen from this example, the answer provided by ChatGPT is very comprehensive. The comment made by ChatGPT about the convergence of the secant method is valuable.

## 2.2 Programming in different languages

In this subsection, we examine the capability of ChatGPT for programming numerical methods in different languages. Specifically, we investigate the languages of C, C++, Python, MATLAB, and Julia. As an example,

we consider the method of successive over-relaxation (SOR) [9, 30, 48], which is an iterative numerical method for solving a system of linear equations $A\vec{x} = \vec{b}$. The numerical procedure for the SOR method is expressed as:

$$x_i^{(k+1)} = (1 - \omega)x_i^{(k)} + \frac{\omega}{a_{ii}} \left( b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k+1)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k)} \right), \tag{2}$$

where $x_i^{(k)}$ represents the $i$-th component of the solution vector at the $k$-th iteration. $a_{ij}$ shows the elements of the matrix $A$. $a_{ii}$ are similarly defined. The elements of the vector $\vec{b}$ are indicated by $b_i$. The number of equations in the system of $A\vec{x} = \vec{b}$ is shown by $n$. $\omega$ stands for the relaxation factor. We ask ChatGPT to develop a code for solving a linear system of equations using the SOR algorithm, respectively, in the languages of MATLAB, C, C++, Python, and Julia. Our dialogues with ChatGPT and resulting codes are listed below.

> **A** Write a MATLAB code for solving a linear system of equations using the method of successive over-relaxation with an example.

> Sure, here's a MATLAB code for solving a linear system of equations using the method of successive over-relaxation with an example:

```matlab
% Successive over-relaxation (SOR) method for solving a linear system of equations
% Ax = b
% Example: solve 4x1 + x2 + x3 = 1, x1 + 4x2 + x3 = 2, x1 + x2 + 4x3 = 3
% using SOR method with omega = 1.5 and tolerance = 1e-6

% Set up the system of equations
A = [4 1 1; 1 4 1; 1 1 4];
b = [1; 2; 3];

% Set up initial guess
x = [0; 0; 0];

% Set up relaxation parameter and tolerance
omega = 1.5;
tol = 1e-6;

% Set up maximum number of iterations
max_iter = 1000;

% Solve the system of equations using SOR method
for iter_count = 1:max_iter
    old_x = x;
    for i = 1:length(x)
        sigma = 0;
        for j = 1:length(x)
            if j ~= i
                sigma = sigma + A(i,j)*x(j);
            end
        end
        x(i) = (1 - omega)*x(i) + (omega/A(i,i))*(b(i) - sigma);
    end
    residual = norm(b - A*x);
    if residual < tol
        break
    end
end

% Display the solution and number of iterations
disp(['Solution:']);
disp(x);
disp(['Number of iterations: ' num2str(iter_count)]);
```

This code sets up the system of equations 'Ax = b' using the matrix **A** and vector 'b', and initializes the initial guess 'x' to be a vector of zeros. The code then uses a loop to perform the SOR method until either the residual is less than the tolerance or the maximum number of iterations is reached. The relaxation parameter 'omega' and tolerance 'tol' are also set at the beginning of the code.

A Write a C code for solving a linear system of equations using the method of successive over-relaxation with an example.

Here's an example of C code for solving a linear system of equations using the method of successive over-relaxation (SOR):

```c
#include <stdio.h>
#include <stdlib.h>
#include <math.h>

#define MAX_ITER 1000

void sor(double **A, double *b, double *x, int n, double omega, double tol) {
    int iter_count = 0;
    double residual = 0.0;
    double *old_x = (double*) malloc(n * sizeof(double));

    do {
        iter_count++;
        residual = 0.0;

        for (int i = 0; i < n; i++) {
            old_x[i] = x[i];
            double sigma = 0.0;

            for (int j = 0; j < n; j++) {
                if (j != i) {
                    sigma += A[i][j] * x[j];
                }
            }

            x[i] = (1.0 - omega) * x[i] + (omega / A[i][i]) * (b[i] - sigma);
            residual += pow(b[i] - A[i][0] * x[0] - A[i][1] * x[1] - A[i][2] * x
[2], 2.0);
        }

        residual = sqrt(residual);

    } while (residual > tol && iter_count < MAX_ITER);

    printf("Solution:\n");
    for (int i = 0; i < n; i++) {
        printf("%.8f ", x[i]);
    }
    printf("\n");

    printf("Number of iterations: %d\n", iter_count);

    free(old_x);
}

int main() {
    double **A = (double**) malloc(3 * sizeof(double*));
    for (int i = 0; i < 3; i++) {
        A[i] = (double*) malloc(3 * sizeof(double));
    }

    A[0][0] = 4.0;
    A[0][1] = 1.0;
```

```
    A[0][2]  = 1.0;
    A[1][0]  = 1.0;
    A[1][1]  = 4.0;
    A[1][2]  = 1.0;
    A[2][0]  = 1.0;
    A[2][1]  = 1.0;
    A[2][2]  = 4.0;

    double b[3] = {1.0, 2.0, 3.0};
    double x[3] = {0.0, 0.0, 0.0};

    double omega = 1.5;
    double tol = 1e-6;

    sor(A, b, x, 3, omega, tol);

    for (int i = 0; i < 3; i++) {
        free(A[i]);
    }
    free(A);

    return 0;
}
```

Write a C++ code for solving a linear system of equations using the method of successive over-relaxation with an example.

Sure, here's an example of C++ code for solving a linear system of equations using the method of successive over-relaxation (SOR):

```cpp
#include <iostream>
#include <cmath>

#define MAX_ITER 1000

using namespace std;

void sor(double **A, double *b, double *x, int n, double omega, double tol) {
    int iter_count = 0;
    double residual = 0.0;
    double *old_x = new double[n];

    do {
        iter_count++;
        residual = 0.0;

        for (int i = 0; i < n; i++) {
            old_x[i] = x[i];
            double sigma = 0.0;

            for (int j = 0; j < n; j++) {
                if (j != i) {
                    sigma += A[i][j] * x[j];
                }
            }

            x[i] = (1.0 - omega) * x[i] + (omega / A[i][i]) * (b[i] - sigma);
            residual += pow(b[i] - A[i][0] * x[0] - A[i][1] * x[1] - A[i][2] * x
[2], 2.0);
        }

        residual = sqrt(residual);

    } while (residual > tol && iter_count < MAX_ITER);
```

```cpp
    cout << "Solution:\n";
    for (int i = 0; i < n; i++) {
        cout << x[i] << " ";
    }
    cout << endl;

    cout << "Number of iterations: " << iter_count << endl;

    delete[] old_x;
}

int main() {
    double **A = new double*[3];
    for (int i = 0; i < 3; i++) {
        A[i] = new double[3];
    }

    A[0][0] = 4.0;
    A[0][1] = 1.0;
    A[0][2] = 1.0;
    A[1][0] = 1.0;
    A[1][1] = 4.0;
    A[1][2] = 1.0;
    A[2][0] = 1.0;
    A[2][1] = 1.0;
    A[2][2] = 4.0;

    double b[3] = {1.0, 2.0, 3.0};
    double x[3] = {0.0, 0.0, 0.0};

    double omega = 1.5;
    double tol = 1e-6;

    sor(A, b, x, 3, omega, tol);

    for (int i = 0; i < 3; i++) {
        delete[] A[i];
    }
    delete[] A;

    return 0;
}
```

A   Write a Python code for solving a linear system of equations using the method of successive over-relaxation with an example.

Sure, here's an example of Python code for solving a linear system of equations using the method of successive over-relaxation (SOR):

```python
import numpy as np

def sor(A, b, x0, omega, tol, max_iter):
    """
    Solves the linear system of equations Ax = b using the method of successive
    over-relaxation (SOR).

    Parameters:
    A (numpy.ndarray): the coefficient matrix of the linear system.
    b (numpy.ndarray): the right-hand side vector of the linear system.
    x0 (numpy.ndarray): the initial guess for the solution vector.
    omega (float): the relaxation parameter.
    tol (float): the tolerance for the residual.
    max_iter (int): the maximum number of iterations.
```

```python
    Returns:
    numpy.ndarray: the solution vector.
    int: the number of iterations performed.
    """

    x = np.copy(x0)
    n = len(x)
    iter_count = 0
    residual = np.linalg.norm(b - A @ x)

    while residual > tol and iter_count < max_iter:
        iter_count += 1
        for i in range(n):
            old_x_i = x[i]
            x[i] += omega * ((b[i] - A[i, :] @ x) / A[i, i] - x[i])
            residual = np.linalg.norm(b - A @ x)
            if residual <= tol:
                break
        if np.allclose(x, old_x_i):
            break

    return x, iter_count

# Define the coefficient matrix A, the right-hand side vector b, and the initial
    guess x0
A = np.array([[4, 1, 1], [1, 4, 1], [1, 1, 4]])
b = np.array([1, 2, 3])
x0 = np.array([0, 0, 0])

# Solve the linear system using SOR
omega = 1.5
tol = 1e-6
max_iter = 1000
x, iter_count = sor(A, b, x0, omega, tol, max_iter)

# Print the solution and the number of iterations
print("Solution:", x)
print("Number of iterations:", iter_count)
```

A Write a Julia code for solving a linear system of equations using the method of successive over-relaxation with an example.

Sure, here's an example of Julia code for solving a linear system of equations using the method of successive over-relaxation (SOR):

```julia
# Successive over-relaxation (SOR) method for solving a linear system of equations
# Ax = b
# Example: solve 4x1 + x2 + x3 = 1, x1 + 4x2 + x3 = 2, x1 + x2 + 4x3 = 3
# using SOR method with omega = 1.5 and tolerance = 1e-6

# Set up the system of equations
A = [4 1 1; 1 4 1; 1 1 4]
b = [1; 2; 3]

# Set up initial guess
x = [0; 0; 0]

# Set up relaxation parameter and tolerance
omega = 1.5
tol = 1e-6

# Set up maximum number of iterations
max_iter = 1000
```

```
# Solve the system of equations using SOR method
for iter_count = 1:max_iter
    old_x = copy(x)
    for i = 1:length(x)
        sigma = 0
        for j = 1:length(x)
            if j != i
                sigma += A[i,j]*x[j]
            end
        end
        x[i] = (1 - omega)*x[i] + (omega/A[i,i])*(b[i] - sigma)
    end
    residual = norm(b - A*x)
    if residual < tol
        break
    end
end

# Display the solution and number of iterations
println("Solution:")
println(x)
println("Number of iterations: ", iter_count)
```

## 2.3  Specifying numerical problems with details

The goal of this subsection is to examine the ability of ChatGPT for solving numerically a given problem with requested details, such as boundary conditions, domain size, etc. As a practical example, we consider the two-dimensional Poisson equation

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = f(x, y), \tag{3}$$

where $\phi(x, y)$ is the scalar variable and $f(x, y)$ is a known source term. To numerically solve the Poisson equation, we discretize the domain into a grid of points and approximate the derivatives using a second-order finite difference method [15, 30, 27]. The resulting discretized equation is written as

$$\frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{\Delta x^2} + \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{\Delta y^2} = f_{i,j}, \tag{4}$$

where $\phi_{i,j}$ is the value of the scalar variable at grid point $(i, j)$, and $\Delta x$ and $\Delta y$ are the grid spacing in the $x$ and $y$ directions, respectively. Additionally, $f_{i,j}$ shows the value of the source term at grid point $(i, j)$.

As a first example, we simply ask ChatGPT to solve the two-dimensional Poisson equation. We do not specify the source term, boundary conditions, domain size, etc. Figure 1 shows the corresponding solution by ChatGPT.

---

**A**  Write a Python code to solve the 2D Poisson equation. Plot the solution.

---

To solve the 2D Poisson equation in Python, we can use the finite difference method, which approximates the differential equations using difference equations that can be solved numerically.
Here's an example Python code that solves the 2D Poisson equation using the finite difference method and plots the solution using Matplotlib:

---

```
import numpy as np
import matplotlib.pyplot as plt

# Define the grid size and spacing
N = 50  # Number of grid points in each direction
L = 1.0  # Length of the square domain
h = L / (N - 1)  # Spacing between grid points

# Define the boundary conditions and source term
u_top = np.zeros(N)
u_bottom = np.zeros(N)
```

```
    u_left = np.zeros(N)
    u_right = np.zeros(N)
    f = np.zeros((N, N))
    f[N//2, N//2] = 1.0/h**2

    # Define the coefficient matrix and the right-hand side vector
    A = np.zeros((N*N, N*N))
    b = np.zeros(N*N)

    for i in range(N):
        for j in range(N):
            k = i*N + j  # Index of the unknown u_ij
            if i == 0:
                A[k, k] = 1.0
                b[k] = u_top[j]
            elif i == N-1:
                A[k, k] = 1.0
                b[k] = u_bottom[j]
            elif j == 0:
                A[k, k] = 1.0
                b[k] = u_left[i]
            elif j == N-1:
                A[k, k] = 1.0
                b[k] = u_right[i]
            else:
                A[k, k] = -4.0
                A[k, k-1] = 1.0
                A[k, k+1] = 1.0
                A[k, k-N] = 1.0
                A[k, k+N] = 1.0
                b[k] = f[i,j]

    # Solve the linear system
    u = np.linalg.solve(A, b)

    # Reshape the solution vector into a 2D array
    U = u.reshape((N, N))

    # Plot the solution
    x = np.linspace(0, L, N)
    y = np.linspace(0, L, N)
    X, Y = np.meshgrid(x, y)
    plt.contourf(X, Y, U)
    plt.colorbar()
    plt.xlabel('x')
    plt.ylabel('y')
    plt.title('2D Poisson equation solution')
    plt.show()
```
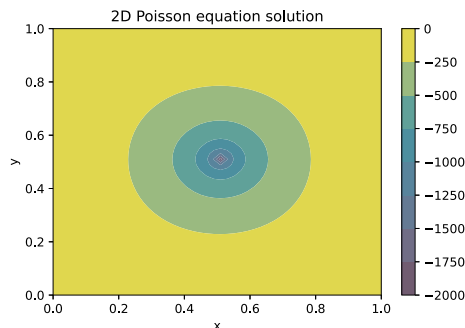


Figure 1: Solution of the Poisson equation (see Eq. 3) by ChatGPT, when we do not specify any detail in our request

As can be observed in Fig. 1, ChatGPT set zero Dirichlet boundary conditions and selected the domain size of $[0, 1] \times [0, 1]$ for solving the Poisson equation (Eq. 3), when we did not specify the details; however, it is not

always the case. One may find another imposed boundary conditions or domain sizes simply by asking the same question from ChatGPT. This is simply because of the fact that ChatGPT has been trained on a large amount of text (and codes can be thought of as a specific type of text).

In the next example, we again ask ChatGPT to solve the two-dimensional Poisson equation; however, we specify the source term to be $f(x, y) = \sin(x) \cos(y)$. Figure 2 depicts the associated output with this request from ChatGPT.

> **A** Write a Python code to solve the 2D Poisson equation with the source term of sin(x)*cos(y). Plot the solution.

> Here's an updated version of the Python code that solves the 2D Poisson equation with the source term of sin(x)*cos(y) and plots the solution using Matplotlib:

```python
import numpy as np
import matplotlib.pyplot as plt

# Define the grid size and spacing
N = 50   # Number of grid points in each direction
L = 1.0   # Length of the square domain
h = L / (N - 1)   # Spacing between grid points

# Define the boundary conditions and source term
u_top = np.zeros(N)
u_bottom = np.zeros(N)
u_left = np.zeros(N)
u_right = np.zeros(N)
x = np.linspace(0, L, N)
y = np.linspace(0, L, N)
X, Y = np.meshgrid(x, y)
f = np.sin(X)*np.cos(Y)

# Define the coefficient matrix and the right-hand side vector
A = np.zeros((N*N, N*N))
b = np.zeros(N*N)

for i in range(N):
    for j in range(N):
        k = i*N + j   # Index of the unknown u_ij
        if i == 0:
            A[k, k] = 1.0
            b[k] = u_top[j]
        elif i == N-1:
            A[k, k] = 1.0
            b[k] = u_bottom[j]
        elif j == 0:
            A[k, k] = 1.0
            b[k] = u_left[i]
        elif j == N-1:
            A[k, k] = 1.0
            b[k] = u_right[i]
        else:
            A[k, k] = -4.0
            A[k, k-1] = 1.0
            A[k, k+1] = 1.0
            A[k, k-N] = 1.0
            A[k, k+N] = 1.0
            b[k] = f[i,j]

# Solve the linear system
u = np.linalg.solve(A, b)

# Reshape the solution vector into a 2D array
U = u.reshape((N, N))

# Plot the solution
plt.contourf(X, Y, U)
```

```
plt.colorbar()
plt.xlabel('x')
plt.ylabel('y')
plt.title('2D Poisson equation solution with sin(x)*cos(y) source term')
plt.show()
```



Figure 2: Solution of the Poisson equation (see Eq. 3) by ChatGPT, when we specify the source term in our request

Eventually, we specify the domain size, boundary condition types, and the source term for solving the two-dimensional Poisson equation. The following chat-box shows our request in details.

> **A** Write a Python code to solve the 2D Poisson equation with the source term of sin(x)*cos(y) in a rectangular domain (centered at the origin) with a length of 5 and a width of 3. Use the zero Dirichlet boundary condition for x=2.5 and x=-2.5. The gradient of the variable is zero on the other boundaries. Plot the solution.

> Here's the Python code to solve the 2D Poisson equation with the source term of sin(x)*cos(y) in a rectangular domain with zero Dirichlet boundary condition for x=2.5 and x=-2.5, and zero Neumann boundary condition for y=-1.5 and y=1.5:

```
import numpy as np
import matplotlib.pyplot as plt

# Define the grid size and spacing
N = 100  # Number of grid points in each direction
Lx = 5.0  # Length of the rectangular domain
Ly = 3.0  # Width of the rectangular domain
h = Lx / (N - 1)  # Spacing between grid points

# Define the boundary conditions and source term
u_top = np.zeros(N)
u_bottom = np.zeros(N)
u_left = np.zeros(N)
u_right = np.zeros(N)
x = np.linspace(-Lx/2, Lx/2, N)
y = np.linspace(-Ly/2, Ly/2, N)
X, Y = np.meshgrid(x, y)
f = np.sin(X)*np.cos(Y)

# Define the coefficient matrix and the right-hand side vector
A = np.zeros((N*N, N*N))
b = np.zeros(N*N)

for i in range(N):
    for j in range(N):
        k = i*N + j  # Index of the unknown u_ij
        if i == 0:
```

```
                A[k, k] = 1.0
                b[k] = u_top[j]
            elif i == N-1:
                A[k, k] = 1.0
                b[k] = u_bottom[j]
            elif j == 0:
                A[k, k] = 1.0
                b[k] = u_left[i]
            elif j == N-1:
                A[k, k] = 1.0
                b[k] = u_right[i]
            elif x[i] == -Lx/2 or x[i] == Lx/2:
                A[k, k] = 1.0
                b[k] = 0.0
            elif y[j] == -Ly/2 or y[j] == Ly/2:
                A[k, k] = -3.0
                if j == 1:
                    A[k, k+N] = 1.0
                    b[k] = 0.0
                elif j == N-2:
                    A[k, k-N] = 1.0
                    b[k] = 0.0
                else:
                    A[k, k-1] = 1.0
                    A[k, k+1] = 1.0
                    b[k] = f[i,j]
            else:
                A[k, k] = -4.0
                A[k, k-1] = 1.0
                A[k, k+1] = 1.0
                A[k, k-N] = 1.0
                A[k, k+N] = 1.0
                b[k] = f[i,j]

# Solve the linear system
u = np.linalg.solve(A, b)

# Reshape the solution vector into a 2D array
U = u.reshape((N, N))

# Plot the solution
plt.contourf(X, Y, U)
plt.colorbar()
plt.xlabel('x')
plt.ylabel('y')
plt.title('2D Poisson equation solution with sin(x)*cos(y) source term')
plt.show()
```
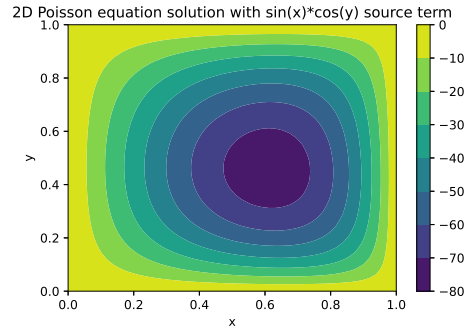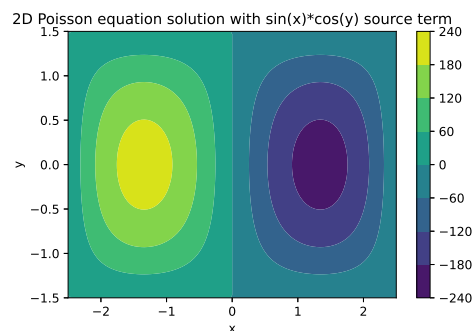


Figure 3: Solution of the Poisson equation (see Eq. 3) by ChatGPT, when we specify the source term and boundary conditions in our request

Looking at our chat box, it is worthwhile to note that we wrote "The gradient of the variable is zero on other boundaries". And ChatGPT wrote in our response: "zero Neumann boundary condition for $y = -1.5$ and $y = 1.5$", which is amazingly exactly equivalent to our request; however, in another wording! Figure 3 exhibits the solution

of the Poisson equation for this case.

## 2.4   The button of "Regenerate response"

There is a "Regenerate response" button in ChatGPT. In this subsection, we investigate the role of this button in generating (programming) codes for a numerical algorithm. For instance, let us consider the diffusion equation. The two-dimensional diffusion equation for a variable $T(x, y, t)$ is written as

$$\frac{\partial T}{\partial t} = D\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + s(x, y, t), \tag{5}$$

where $D$ is the diffusion coefficient and $s(x, y, t)$ is a known source term. To numerically solve the two-dimensional diffusion, we might use the forward-time central space (FTCS) method [15], which approximates the derivatives in time and space using a central difference approximation as follows

$$\frac{\partial T}{\partial t} \approx \frac{T_{i,j}^{n+1} - T_{i,j}^{n}}{\Delta t}, \tag{6}$$

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T_{i+1,j}^{n} - 2T_{i,j}^{n} + T_{i-1,j}^{n}}{\Delta x^2}, \tag{7}$$

$$\frac{\partial^2 T}{\partial y^2} \approx \frac{T_{i,j+1}^{n} - 2T_{i,j}^{n} + T_{i,j-1}^{n}}{\Delta y^2}, \tag{8}$$

where $T_{i,j}^{n}$ is the value at grid point $(i, j)$ and time step $n$. Additionally, $\Delta x$, $\Delta y$, and $\Delta t$ are the grid spacing in the $x$ and $y$ directions and the time step, respectively. Substituting these approximations into the two-dimensional diffusion equation and rearranging, we obtain a finite difference equation for the value of $T_{i,j}^{n+1}$

$$T_{i,j}^{n+1} = T_{i,j}^{n} + D\frac{\Delta t}{\Delta x^2}(T_{i+1,j}^{n} - 2T_{i,j}^{n} + T_{i-1,j}^{n}) + D\frac{\Delta t}{\Delta y^2}(T_{i,j+1}^{n} - 2T_{i,j}^{n} + T_{i,j-1}^{n}) + s_{i,j}^{n}\Delta t, \tag{9}$$

where $s_{i,j}^{n}$ is the value of the source term at grid point $(i, j)$. The FTCS method is numerically stable if and only if the following condition is satisfied

$$\Delta t \leq \frac{1}{2D}\frac{1}{\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right)}. \tag{10}$$

Now we ask ChatGPT to numerically solve the two-dimensional diffusion equation (Eq. 5) using the FTCS method (see Eq. 9).

---

**A**  Write a Python code for solving the 2D diffusion equation in a square box using the FTCS (Forward Time Centered Space) method. Use Dirichlet boundary conditions such that the value of the variable is 0 on the right and left boundaries, while they are 1 on the top and bottom.

---

Here is a Python code for solving the 2D diffusion equation in a square box using the FTCS method:

---

```python
import numpy as np
import matplotlib.pyplot as plt

# Define the parameters
D = 0.1   # Diffusion coefficient
L = 1.0   # Length of the square box
N = 100   # Number of grid points in each direction
dx = L / (N - 1)   # Grid spacing
dy = L / (N - 1)
dt = 0.0001   # Time step
t_final = 1.0   # Final time

# Define the initial condition
u = np.zeros((N, N))
u[:, 0] = 1.0   # Bottom boundary
u[:, -1] = 1.0   # Top boundary
u[0, :] = 0.0   # Left boundary
u[-1, :] = 0.0   # Right boundary

# Define the coefficients for the FTCS method
alpha = D * dt / dx**2
```

```
    beta = D * dt / dy**2

    # Iterate in time
    t = 0.0
    while t < t_final:
        # Compute the next time step
        u[1:-1, 1:-1] += alpha * (u[2:, 1:-1] - 2*u[1:-1, 1:-1] + u[:-2, 1:-1]) + beta
        * (u[1:-1, 2:] - 2*u[1:-1, 1:-1] + u[1:-1, :-2])

        # Update the boundary conditions
        u[:, 0] = 1.0  # Bottom boundary
        u[:, -1] = 1.0  # Top boundary
        u[0, :] = 0.0  # Left boundary
        u[-1, :] = 0.0  # Right boundary

        # Increase the time
        t += dt

    # Plot the solution
    x = np.linspace(0, L, N)
    y = np.linspace(0, L, N)
    X, Y = np.meshgrid(x, y)
    plt.pcolormesh(X, Y, u, cmap='coolwarm')
    plt.colorbar()
    plt.xlabel('x')
    plt.ylabel('y')
    plt.title('Diffusion equation in a square box')
    plt.show()
```



Figure 4: Solution of the two-dimensional diffusion equation (see Eq. 5) using the FTCS method (see Eq. 9) by ChatGPT

After receiving this response from ChatGPT, we immediately press the "Regenerate response" button. We receive the following response (i.e., code).

```
import numpy as np
import matplotlib.pyplot as plt

# Define the parameters
D = 1.0  # diffusion coefficient
L = 1.0  # size of the square box
Nx = 51  # number of grid points in the x direction
Ny = 51  # number of grid points in the y direction
dx = L/(Nx-1)  # grid spacing in the x direction
dy = L/(Ny-1)  # grid spacing in the y direction
dt = 0.0001  # time step
T = 1.0  # final time

# Define the initial conditions
u = np.zeros((Nx,Ny))
u[:,0] = 1.0  # Dirichlet boundary condition at the bottom
u[:,-1] = 1.0  # Dirichlet boundary condition at the top
```

```
    u[0,:] = 0.0  # Dirichlet boundary condition on the left
    u[-1,:] = 0.0  # Dirichlet boundary condition on the right

    # Define the FTCS scheme
    def ftcs(u, D, dx, dy, dt):
        Nx, Ny = u.shape
        u_new = u.copy()
        for i in range(1, Nx-1):
            for j in range(1, Ny-1):
                u_new[i,j] = u[i,j] + D*dt*(u[i+1,j] - 2*u[i,j] + u[i-1,j])/dx**2 \
                            + D*dt*(u[i,j+1] - 2*u[i,j] + u[i,j-1])/dy**2
        return u_new

    # Solve the diffusion equation using the FTCS scheme
    t = 0.0
    while t < T:
        u = ftcs(u, D, dx, dy, dt)
        t += dt

    # Plot the results
    x = np.linspace(0, L, Nx)
    y = np.linspace(0, L, Ny)
    X, Y = np.meshgrid(x, y)
    plt.contourf(X, Y, u, cmap='coolwarm')
    plt.colorbar()
    plt.xlabel('x')
    plt.ylabel('y')
    plt.title('Diffusion in a Square Box')
    plt.show()
```
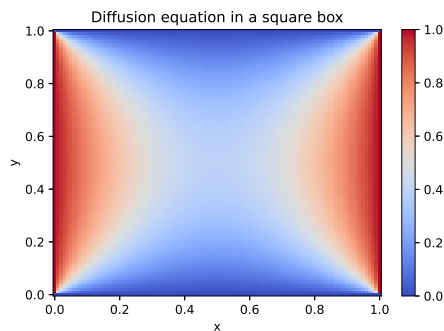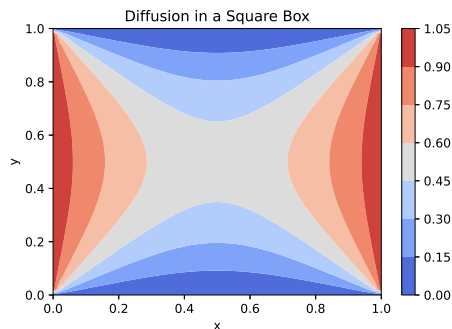


Figure 5: Solution of the two-dimensional diffusion equation (see Eq. 5) using the FTCS method (see Eq. 9) by ChatGPT after pressing the button of "Regenerate response"

Comparing these two codes, we realize that they have completely different structures. In fact, it seems that the machine has been massively trained over a variety of texts. However, in terms of performance, there is no significant difference between these two codes. Another possible question is that if one presses the button of "Regenerate response" again, what the ChatGPT output would be, or how many different responses ChatGPT can generate for a unique question?!

## 2.5   One-dimensional compressible inviscid flow

We so far asked ChatGPT to program numerical solvers for a single partial differential equation such as the Poisson equation and the diffusion equation. In this subsection, we explore the capability of ChatGPT for more complicated partial differential equations. A valuable example is the Euler equations governing the one-dimensional compressible inviscid flow [28, 13]. Because there is an exact solution to this problem [11, 16], it is widely used as a standard test case for the validation of numerical solvers. The equations of the conservation of mass, momentum, and energy in the $x$ direction for one-dimensional compressible inviscid flow are, respectively, written as

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_x)}{\partial x} = 0, \tag{11}$$

16

$$\frac{\partial(\rho u_x)}{\partial t} + \frac{\partial(\rho u_x^2 + p)}{\partial x} = 0, \tag{12}$$

$$\frac{\partial E}{\partial t} + \frac{\partial(E u_x + p u_x)}{\partial x} = 0, \tag{13}$$

where $\rho$ shows the density. The velocity in the $x$ direction is indicated by $u_x$. The pressue is shown by $p$. Additionally, $E$ is the total energy per unit volume and is expressed as

$$E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho u_x^2, \tag{14}$$

where $\gamma$ is the specific heat ratio. We ask ChatGPT to write a code for us for obtaining a numerical solution to this problem.

> **A** Write a Matlab code for solving 1D compressible Euler equation with an example that shock happens.

> Sure, here's a Matlab code for solving the 1D compressible Euler equations using the Godunov method, with an example that generates a shock wave:

```matlab
% Parameters
gamma = 1.4; % Ratio of specific heats
N = 1000; % Number of grid points
L = 1; % Length of the domain
dx = L/N; % Grid spacing
dt = 0.00001; % Time step
t_final = 0.2; % Final time

% Initial conditions
x = linspace(0, L, N);
rho = ones(1, N);
rho(x>0.5) = 0.125;
u = zeros(1, N);
p = ones(1, N);
p(x>0.5) = 0.1;
E = p/(gamma-1) + 0.5*rho.*u.^2;

% Godunov method
t = 0;
while t < t_final
    % Compute time step
    a = sqrt(gamma*p./rho);
    dt = 0.25*dx./(abs(u) + a);
    dt = min(dt);
    if t + dt > t_final
        dt = t_final - t;
    end

    % Compute fluxes
    f = zeros(3, N+1);
    for i = 1:N+1
        if i == 1
            f(:, i) = euler_flux(rho(1), u(1), p(1), gamma);
        elseif i == N+1
            f(:, i) = euler_flux(rho(end), u(end), p(end), gamma);
        else
            f(:, i) = riemann_solver(rho(i-1), u(i-1), p(i-1), rho(i), u(i), p(i), gamma);
        end
    end

    % Update solution
    rho = rho - dt/dx*(f(1, 2:end) - f(1, 1:end-1));
    u = u - dt/dx*(f(2, 2:end) - f(2, 1:end-1));
    E = E - dt/dx*(f(3, 2:end) - f(3, 1:end-1));
    p = (gamma-1)*(E - 0.5*rho.*u.^2);
```

```matlab
    % Boundary conditions
    rho(1) = rho(2);
    rho(end) = rho(end-1);
    u(1) = -u(2);
    u(end) = -u(end-1);

    % Update time
    t = t + dt;
end

% Plot solution
figure;
plot(x, rho, 'b', 'LineWidth', 2);
xlabel('x');
ylabel('Density');
title('1D Compressible Euler Equations with a Shock Wave');
xlim([0 L]);

figure;
plot(x, u, 'b', 'LineWidth', 2);
xlabel('x');
ylabel('Velocity');
title('1D Compressible Euler Equations with a Shock Wave');
xlim([0 L]);

figure;
plot(x, p, 'b', 'LineWidth', 2);
xlabel('x');
ylabel('Pressure');
title('1D Compressible Euler Equations with a Shock Wave');
xlim([0 L]);

% Function to compute Euler fluxes
function f = euler_flux(rho, u, p, gamma)
    f = [rho*u; rho*u^2 + p; (p/(gamma-1) + 0.5*rho*u^2 + p)*u];
end

% Function to compute Riemann fluxes
function f = riemann_solver(rho_l, u_l, p_l, rho_r, u_r, p_r, gamma)
    % Compute left and right state variables
    c_l = sqrt(gamma*p_l/rho_l);
    c_r = sqrt(gamma*p_r/rho_r);
    rho_star = 0.5*(rho_l + rho_r) + 0.5*(u_l - u_r)/c_l/sqrt(2/gamma/(gamma-1)/
    rho_l + 2/gamma/(gamma-1)/rho_r);
    p_star = 0.5*(p_l + p_r) + 0.5*(u_l - u_r)*rho_star*c_l;
    if p_star < 0
        p_star = 0;
    end
    u_star = 0.5*(u_l + u_r) + 0.5*(p_l - p_r)/rho_star/c_l;

    % Compute left and right wave speeds
    s_l = u_star - c_l;
    s_r = u_star + c_r;

    % Compute Euler fluxes at left and right states
    f_l = euler_flux(rho_l, u_l, p_l, gamma);
    f_r = euler_flux(rho_r, u_r, p_r, gamma);

    % Compute total energy per unit volume at the right state
    E_r = p_r/(gamma-1) + 0.5*rho_r*u_r^2;
    E_l = p_l/(gamma-1) + 0.5*rho_l*u_l^2;

    % Compute numerical flux
    if s_l > 0
        f = euler_flux(rho_l, u_l, p_l, gamma);
    elseif s_r < 0
        f = euler_flux(rho_r, u_r, p_r, gamma);
    else
        f = zeros(3, 1);
        f(1) = (s_r*f_l(1) - s_l*f_r(1) + s_l*s_r*(rho_r - rho_l))/(s_r - s_l);
```

```
    f(2) = (s_r*f_l(2) - s_l*f_r(2) + s_l*s_r*(rho_r*u_r - rho_l*u_l))/(s_r -
s_l) + (p_star - 0.5*(rho_l + rho_r)*(s_r - s_l))*0.5*(sign(s_l) + sign(s_r));
    f(3) = (s_r*f_l(3) - s_l*f_r(3) + s_l*s_r*(rho_r*E_r - rho_l*E_l))/(s_r -
s_l) + (p_star*u_star - 0.5*(rho_l*u_l + rho_r*u_r)*(s_r - s_l))*0.5*(sign(s_l)
 + sign(s_r));
    end
end
```
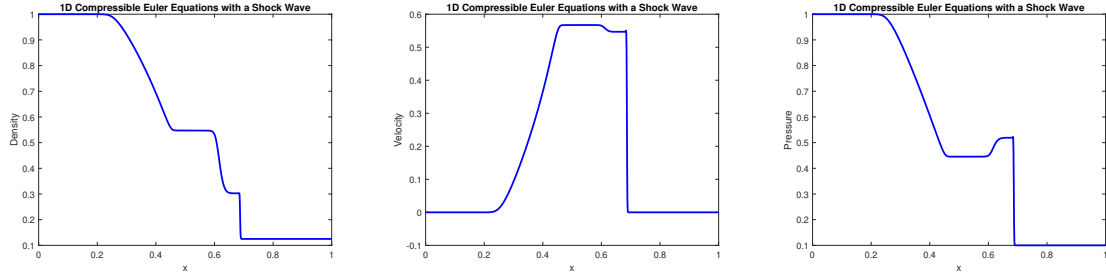


Figure 6: Numerical solutions (using the Godunov method) of the density, velocity, and pressure variables for the one-dimensional compressible inviscid flow (see Eqs. 11–13) for the Sod shock tube problem by the MATLAB code generated by ChatGPT

Note that ChatGPT considered the representative test case of the Sod shock tube problem [42] to validate the generated code. The numerical solutions of the density, velocity, and pressure fields obtained by the MATLAB code generated by ChatGPT are plotted in Fig. 6. Additionally, we plot the exact solutions for these three variables in Fig. 7. By comparing Fig. 6 and Fig 7, it is realized that although the general trend of the numerical solution is correct, there are significant errors in estimating the correct positions of contact discontinuity and shock discontinuity. However, these errors are due to the Godunov method. One may ask ChatGPT to generate the relevant codes using more accurate numerical methods for solving compressible flow equations.
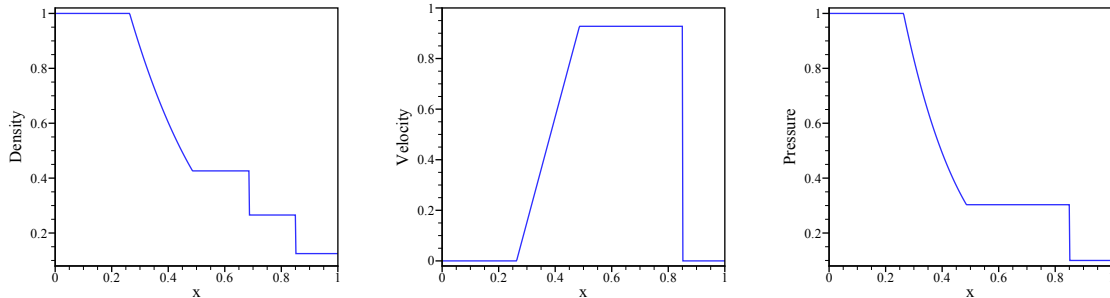


Figure 7: Exact solutions of the density, velocity, and pressure variables for the one-dimensional compressible inviscid flow (see Eqs. 11–13) for the Sod shock tube problem

# 3   Machine learning for computational physics by ChatGPT

## 3.1   Physics-informed neural networks (PINNs)

Physics-informed neural networks (PINNs) [37, 47, 23, 24] are specific neural networks used in scientific machine learning to predict the solution of partial differential equations of physical systems. The key feature of PINNs is to impose the residual of partial differential equations into the loss function. In this way, by minimizing the loss, the outputs of PINNs satisfy the governing equations. In simple words, PINNs are neural networks that learn from the boundary and initial conditions as well as the underlying physics to solve a forward problem. Alternatively, PINNs can be used to solve an inverse problem by learning from sparse data as well as the underlying physics.

In this subsection, for example, we ask ChatGPT to solve a forward problem using the PINN methodology. Particularly, we consider the one-dimensional diffusion equation for the variable $\theta(x,t)$ with the source term as

follows

$$\frac{\partial\theta}{\partial t} = \frac{\partial^2\theta}{\partial x^2} + \cos(x)\big(\cos(t) - \sin(t)\big), \tag{15}$$

which has an exact analytical solution of $\theta(x,t) = \cos(x)\cos(t)$. Boundary and initial conditions of Eq. 15 obey the exact solution. According to the PINN methodology, the loss function ($\mathcal{L}$) is defined as

$$\mathcal{L} = \frac{1}{M_1}\sum_{i=1}^{M_1}\big(\hat{\theta}_i - \theta_i^{\mathrm{bc}}\big)^2 + \frac{1}{M_2}\sum_{i=1}^{M_2}\big(\hat{\theta}_i - \theta_i^{\mathrm{ic}}\big)^2 + \frac{1}{N}\sum_{i=1}^{N}\bigg(\frac{\delta\hat{\theta}_i}{\delta t_i} - \frac{\delta}{\delta x_i}\Big(\frac{\delta\hat{\theta}_i}{\delta x_i}\Big) - \cos(x_i)\big(\cos(t_i) - \sin(t_i)\big)\bigg)^2, \tag{16}$$

where $\delta$ indicates the automatic differentiation operator in Tensorflow [1]. $\hat{\theta}$ is the value predicted by PINN. $\theta^{\mathrm{bc}}$ and $\theta^{\mathrm{ic}}$ show the value of $\theta(x,t)$ at the boundary and initial points, respectively. The number of points located at the boundary and initial conditions are respectively indicated by $M_1$ and $M_2$. $N$ is the number of interior points of the domain. We ask ChatGPT to find the solution to this partial differential equation (Eq. 15) using PINN.

---

**A** Write a Python code for finding the solution of the partial differential equation of u_t = u_xx + cos(x)*(cos(t)-sin(t)) using the PINN methodology. The neural network is only aware of the boundary and initial conditions, which obey the exact solution of u(x,t) = cos(x)*cos(t). Plot the exact solution and the predicted solution.

---

To solve the given partial differential equation (PDE) using the Physics-Informed Neural Networks (PINN) methodology, we'll follow these steps:

1. Import the necessary libraries.

2. Define the neural network architecture.

3. Set up the boundary and initial conditions.

4. Train the neural network.

5. Evaluate and plot the results.

Here's a Python code implementing the PINN methodology for the given PDE:

---

```python
import tensorflow.compat.v1 as tf
tf.disable_v2_behavior()
import numpy as np
import matplotlib.pyplot as plt

# Define the computational graph
graph = tf.Graph()
with graph.as_default():
    # Define the input tensors
    x = tf.placeholder(tf.float32, [None, 1], name='x')
    t = tf.placeholder(tf.float32, [None, 1], name='t')
    u = tf.placeholder(tf.float32, [None, 1], name='u')

    # Define the neural network architecture
    with tf.variable_scope('neural_net'):
        h1 = tf.layers.dense(tf.concat([x, t], axis=1), 50, activation=tf.nn.tanh)
        h2 = tf.layers.dense(h1, 50, activation=tf.nn.tanh)
        h3 = tf.layers.dense(h2, 50, activation=tf.nn.tanh)
        pred = tf.layers.dense(h3, 1, activation=None, name='pred')

    # Define the loss function
    with tf.variable_scope('loss'):
        # Define the PDE residual
        u_x, u_t = tf.gradients(pred, [x, t])
        u_xx = tf.gradients(u_x, [x])
        f = u_t - u_xx - tf.cos(x)*(tf.cos(t)-tf.sin(t))

        # Define the boundary conditions
        bc_left = tf.reduce_mean(tf.square(pred[:, 0] - u[:, 0]))
        bc_right = tf.reduce_mean(tf.square(pred[:, -1] - u[:, -1]))
```

```python
        # Define the total loss
        loss = bc_left + bc_right + tf.reduce_mean(tf.square(f))

    # Define the optimizer
    with tf.variable_scope('optimizer'):
        optimizer = tf.train.AdamOptimizer().minimize(loss)

# Define the exact solution
def exact_solution(x, t):
    return np.cos(x)*np.cos(t)

# Define the initial and boundary conditions
def initial_condition(x,t):
    return np.cos(x)*np.cos(t)

def boundary_condition(x,t):
    return np.cos(x)*np.cos(t)

# Train the neural network
with tf.Session(graph=graph) as sess:
    sess.run(tf.global_variables_initializer())

    # Generate some training data
    x_train =  np.random.uniform(-1, 1, (5000, 1))
    t_train =  np.random.uniform(0, 1, (5000, 1))
    u_train = exact_solution(x_train, t_train)

    # Set the initial and boundary conditions
    u_train[:, 0] = initial_condition(x_train[:, 0], t_train[:, 0])
    u_train[:, -1] = boundary_condition(x_train[:, 0] , t_train[:, 0])

    # Train the neural network
    for i in range(1000):
        _, loss_val = sess.run([optimizer, loss], feed_dict={x: x_train, t: t_train
    , u: u_train})

        if i % 100 == 0:
            print('Step {}: loss = {}'.format(i, loss_val))

    # Evaluate the neural network on the test data
    u_pred_val = sess.run(pred, feed_dict={x: x_train, t: t_train})

    # Print the mean squared error
    mse = np.mean(np.square(u_train - u_pred_val))
    print('Mean squared error: {}'.format(mse))

    plt.figure(figsize=(6, 6))
    plt.scatter(x_train, t_train, 0.1, color='blue', label='Training points')
    plt.xlabel('x')
    plt.ylabel('t')
    plt.title('Location of training points')
    plt.show()

    # Define the grid
    x = np.linspace(-1, 1, 100)
    t = np.linspace(0, 1, 100)
    X, T = np.meshgrid(x, t)

    # Compute the exact solution on the grid
    U = exact_solution(X, T)

    # Plot the contour of the solution
    plt.contourf(X, T, U,cmap='jet')
    plt.colorbar()
    plt.xlabel('x')
    plt.ylabel('t')
    plt.title('Exact Solution')
    plt.show()

    # Plot the contour of the prediction
    plt.scatter(x_train, t_train, 1.0, u_pred_val[:,0], cmap='jet')
```

```
        cbar= plt.colorbar()
        plt.xlabel('x')
        plt.ylabel('t')
        plt.title('Predicted Solution')
        plt.show()
```
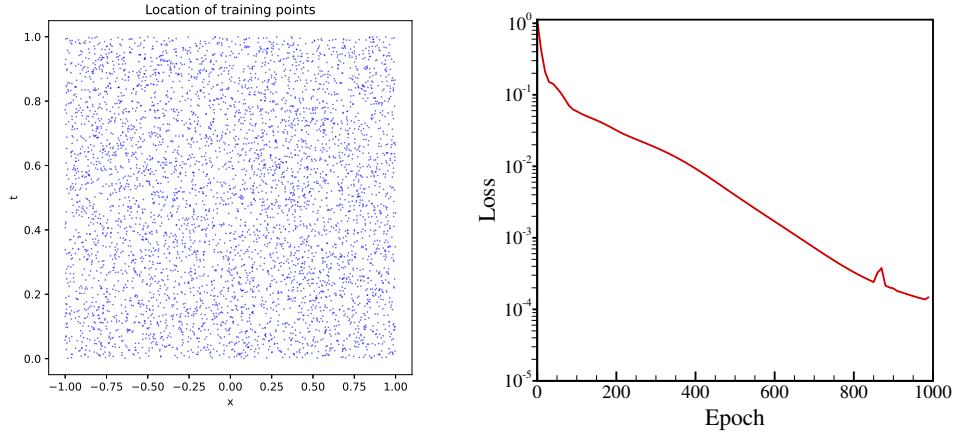


Figure 8: Location of training points (left) and loss ($\mathcal{L}$) history (right) for solving the partial differential equation (Eq. 15) by ChatGPT using the PINN methodology
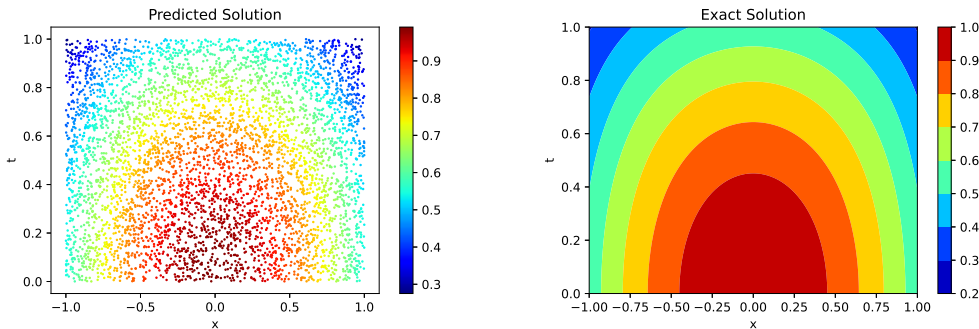


Figure 9: A comparison between the exact solution and the predicted solution to the partial differential equation (Eq. 15) generated by ChatGPT

## 3.2  Convolutional neural networks (CNNs) for computational physics

Convolutional neural networks (CNNs) are among popular artificial neural networks widely used for image classification and image segmentation purposes in computer visions and computer graphics, due to their capabilities for pattern recognition. In this sense, CNNs can be used for supervised learning of computational mechanics, when the problem solution is a function of geometric parameters [3, 45]. In this approach, the data must be represented on Cartesian grids (i.e., image-like data). For example, we can design a deep learning framework, where the CNN input is the images of airfoils with different shapes and the CNN output is the velocity and pressure fields. We ask ChatGPT to develop a Python code for designing a CNN-based deep learning framework to predict the flow fields around airfoils.

> **A** Develop a Python code for the prediction of the velocity and pressure fields around airfoils with different geometries in two dimensions. Specifically, use convolutional neural networks to encode geometric features and then use deconvolutional neural networks to decode the outputs. Input is 128 by 128 images, and the output has the same size.

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To predict the velocity and pressure fields around two-dimensional airfoils with different geometries using a combination of convolutional neural networks (CNNs) and deconvolutional neural networks (also known as transposed convolutions), you can follow these steps:

1. Data preparation: Obtain a dataset with airfoil shapes and corresponding velocity and pressure fields. You can use computational fluid dynamics (CFD) simulations or experimental data for this purpose.

2. Data preprocessing: Normalize and resize the airfoil images and velocity and pressure fields to a suitable size for the CNN. Split the dataset into training, validation, and test sets.

3. Model creation: Design a CNN architecture for encoding geometric features and a deconvolutional neural network for decoding the outputs.

4. Training: Train the combined model using the training and validation datasets.

5. Testing: Evaluate the model's performance on the test dataset.

Here's a sample code using TensorFlow and Keras:

```python
import tensorflow as tf
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Conv2D, MaxPooling2D, Dense, Flatten, Dropout,
    Conv2DTranspose, UpSampling2D, BatchNormalization
from tensorflow.keras.optimizers import Adam
import numpy as np
import os

def load_data(path):
    # Load your dataset here
    pass

def preprocess_data(data):
    # Preprocess your data here (normalize, resize, split)
    pass

def create_model(input_shape):
    model = Sequential()

    # Encoder
    model.add(Conv2D(32, (3, 3), activation='relu', padding='same', input_shape=
    input_shape))
    model.add(MaxPooling2D((2, 2), padding='same'))
    model.add(Conv2D(64, (3, 3), activation='relu', padding='same'))
    model.add(MaxPooling2D((2, 2), padding='same'))
    model.add(Conv2D(128, (3, 3), activation='relu', padding='same'))
    model.add(MaxPooling2D((2, 2), padding='same'))

    # Decoder
    model.add(Conv2DTranspose(128, (3, 3), activation='relu', padding='same'))
    model.add(UpSampling2D((2, 2)))
    model.add(Conv2DTranspose(64, (3, 3), activation='relu', padding='same'))
    model.add(UpSampling2D((2, 2)))
    model.add(Conv2DTranspose(32, (3, 3), activation='relu', padding='same'))
    model.add(UpSampling2D((2, 2)))
    model.add(Conv2DTranspose(3, (3, 3), activation='linear', padding='same'))  # 3
     channels for u, v velocity components and pressure

    return model

def train_model(model, train_data, val_data, epochs, batch_size):
    model.compile(optimizer=Adam(learning_rate=0.001),
                  loss='mse',
                  metrics=['mae'])

    history = model.fit(train_data,
                        epochs=epochs,
                        batch_size=batch_size,
                        validation_data=val_data)

    return history, model
```

```python
    def test_model(model, test_data):
        # Evaluate the model on the test dataset
        pass

    if __name__ == '__main__':
        # Load and preprocess the data
        dataset_path = "path/to/your/dataset"
        data = load_data(dataset_path)
        train_data, val_data, test_data = preprocess_data(data)

        # Create the CNN model
        input_shape = (128, 128, 1)  # Input shape based on your preprocessed data
        model = create_model(input_shape)

        # Train the model
        epochs = 50
        batch_size = 32
        history, trained_model = train_model(model, train_data, val_data, epochs,
        batch_size)

        # Test the model
        test_results = test_model(trained_model, test_data)
```

This sample code provides a starting point for your project. You'll need to implement the functions to load and preprocess the data, as well as modify the CNN architecture and parameters according to your specific dataset and requirements.

There are two notable observations. First, ChatGPT implements the "mean squared error" as the loss function in line 40 of the above code. This is interesting because although this is an image-based prediction problem, ChatGPT realizes that this is, indeed, a regression task. Line 40 of the above code is listed below as well.

```python
    def train_model(model, train_data, val_data, epochs, batch_size):
        model.compile(optimizer=Adam(learning_rate=0.001),
                      loss='mse',
                      metrics=['mae'])
```

Second, ChatGPT implements the last layer of the network with three outputs for the velocity in the $x$ and $y$ directions and the pressure, as can be seen in line 34 of the above code, showing that GPT understands that the velocity field in two dimensions is a vector with two components and the pressure is simply a scalar variable. Line 34 of the above code is listed below as well.

```python
    model.add(Conv2DTranspose(3, (3, 3), activation='linear', padding='same'))  # 3
        channels for u, v velocity components and pressure
```

# 4   Debugging and improving codes using ChatGPT

In this subsection, we investigate if ChatGPT can help us debug and improve our codes. As a practical example, we consider the Gauss-Seidel method [48]. The Gauss-Seidel algorithm is used for obtaining a numerical solution to a system of linear equations $A\vec{x} = \vec{b}$. Given an initial guess such as the vector $\vec{x}^{(0)}$, the solution can be approximated using the following formula iteratively:

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left( b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k+1)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k)} \right), \tag{17}$$

where $x_i^{(k)}$ indicates the $i$-th component of the solution vector at the $k$-th iteration, $a_{ij}$ show the coefficients of the matrix $A$, and $b_i$ denotes the constants in the vector $\vec{b}$. We test ChatGPT with a C++ code written by the first author (A. Kashefi) that solves the system of $A\vec{x} = \vec{b}$. We provide ChatGPT with the code and ask if the code produces the correct results.

I have written a C++ code for solving a system of equations using the Gauss-Seidel method. The code is as follows. Please let me know if the output of the code is correct.

```cpp
#define _USE_MATH_DEFINES
#include <iostream>
#include <fstream>
#include <sstream>
#include <math.h>

using namespace std ;

void GS(double **a, double x[], double b[], int n){

  double *r = new double[n] ;
  double *xK = new double[n] ;

  for(int j = 0 ; j < n ; j++){r[j] = 0 ; xK[j] = 0; x[j] = 0;}

  while(true){

    for(int i = 0 ; i < n ; i ++){

      double sum1 = 0;
      double sum2 = 0;

      for(int j = 0 ; j < i ; j++){if(i==0){sum1 = 0 ; break ;}
        sum1 += a[i][j]*xK[j] ;}

      for(int j = i+1 ; j < n ; j++)
        sum2 += a[i][j]*x[j] ;

      xK[i] = (1./a[i][i])*(b[i] - sum1 - sum2);
    }

    for(int i = 0 ; i < n ; i ++){x[i] = xK[i];}

    for(int i = 0 ; i < n ; i ++){

      double sum = 0 ;
      for(int k = 0 ; k < n ; k ++)
        sum += a[i][k]*x[k] ;

      r[i] = b[i] - sum ;
    }

    double max = 0 ;
    for(int i = 0 ; i < n ; i ++){if(abs(r[i]) > max){max = abs(r[i]);}}
    if(max < pow(10. , -6.)){break ;}
  }

  return ;
}

int main(){

    // Formulate the problem as Ax = b

  int n = 5 ;
  double *b, *x ;
  b = new double[n] ;
  x = new double[n] ;

  double** a = new double*[n] ;
  for (int i = 0 ; i < n ; i++)
    a[i] = new double[n];

  // As an example
```

```
    b[0]  =  4. ;
    b[1]  =  24. ;
    b[2]  =  8. ;
    b[3]  =  5. ;
    b[4]  =  24. ;

    a[0][0]=6; a[0][1]=2; a[0][2]=3 ; a[0][3]=4 ; a[0][4]=1 ;
    a[1][0]=2 ; a[1][1]=6 ; a[1][2]=2 ; a[1][3]=3 ; a[1][4]=4 ;
    a[2][0]=3 ; a[2][1]=2 ; a[2][2]=6 ; a[2][3]=2 ; a[2][4]=3 ;
    a[3][0]=4 ; a[3][1]=3 ; a[3][2]=2 ; a[3][3]=6 ; a[3][4]=2 ;
    a[4][0]=1 ; a[4][1]=4 ; a[4][2]=3 ; a[4][3]=2 ; a[4][4]=6 ;

    GS(a, x, b, n) ;

    for(int i=0; i<n ; i++){cout << "x" << i << "  " << x[i] << endl ;}
    return 0;
}
```

The code for solving a system of equations using the Gauss-Seidel method looks fine. However, to check whether the output of the code is correct, we need to compare it with the actual solution.
For the given system of equations:

```
6x1 + 2x2 + 3x3 + 4x4 + 1x5 = 4
2x1 + 6x2 + 2x3 + 3x4 + 4x5 = 24
3x1 + 2x2 + 6x3 + 2x4 + 3x5 = 8
4x1 + 3x2 + 2x3 + 6x4 + 2x5 = 5
1x1 + 4x2 + 3x3 + 2x4 + 6x5 = 24
```

The actual solution is x1 = 1, x2 = 2, x3 = 1, x4 = -1, and x5 = 3.
Running the provided code, we get the following output:

```
x0   1.00003
x1   1.99994
x2   0.999965
x3   -0.999985
x4   2.99997
```

The We can see that the output of the code is very close to the actual solution. The small differences may be due to numerical error, and can be reduced by increasing the number of iterations or using double precision arithmetic.
Therefore, the output of the code is correct.

ChatGPT could surprisingly successfully recognize the embedded system of equations ($A\vec{x} = \vec{b}$) inside our C++ code (see lines 64 to 76 of the above code). Additionally, it seems that ChatGPT ran our code (using perhaps an inner compiler) as it said in the chat box: "Running the provided code, we get the following output".

For the next step, we intentionally put a bug in our C++ code. In the loop written in line 18 of the following code, we start indexing from "10" instead of "0", and we ask the same question from ChatGPT.

A   I have written a C++ code for solving a system of equations using the Gauss-Seidel method. The code is as follows. Please let me know if the code works correctly or not!

```
#define _USE_MATH_DEFINES
#include <iostream>
#include <fstream>
```

```cpp
#include <sstream>
#include <math.h>

using namespace std ;

void GS(double **a, double x[], double b[], int n){

  double *r = new double[n] ;
  double *xK = new double[n] ;

  for(int j = 0 ; j < n ; j++){r[j] = 0 ; xK[j] = 0; x[j] = 0;}

  while(true){

    for(int i = 10 ; i < n ; i ++){

      double sum1 = 0;
      double sum2 = 0;

      for(int j = 0 ; j < i ; j++){if(i==0){sum1 = 0 ; break ;}
        sum1 += a[i][j]*xK[j] ;}

      for(int j = i+1 ; j < n ; j++)
        sum2 += a[i][j]*x[j] ;

      xK[i] = (1./a[i][i])*(b[i] - sum1 - sum2);
    }

    for(int i = 0 ; i < n ; i ++){x[i] = xK[i];}

    for(int i = 0 ; i < n ; i ++){

      double sum = 0 ;
      for(int k = 0 ; k < n ; k ++)
        sum += a[i][k]*x[k] ;

      r[i] = b[i] - sum ;
    }

    double max = 0 ;
    for(int i = 0 ; i < n ; i ++){if(abs(r[i]) > max){max = abs(r[i]);}}
    if(max < pow(10. , -6.)){break ;}
  }

  return ;
}

int main(){

    // Formulate the problem as Ax = b

  int n = 5 ;
  double *b, *x ;
  b = new double[n] ;
  x = new double[n] ;

  double** a = new double*[n] ;
  for (int i = 0 ; i < n ; i++)
    a[i] = new double[n];

  // As an example

  b[0] = 4. ;
  b[1] = 24. ;
  b[2] = 8. ;
  b[3] = 5. ;
  b[4] = 24. ;

  a[0][0]=6; a[0][1]=2; a[0][2]=3 ; a[0][3]=4 ; a[0][4]=1 ;
  a[1][0]=2 ; a[1][1]=6 ; a[1][2]=2 ; a[1][3]=3 ; a[1][4]=4 ;
  a[2][0]=3 ; a[2][1]=2 ; a[2][2]=6 ; a[2][3]=2 ; a[2][4]=3 ;
```

```
    a[3][0]=4 ; a[3][1]=3 ; a[3][2]=2 ; a[3][3]=6 ; a[3][4]=2 ;
    a[4][0]=1 ; a[4][1]=4 ; a[4][2]=3 ; a[4][3]=2 ; a[4][4]=6 ;

    GS(a, x, b, n) ;

    for(int i=0; i<n ; i++){cout << "x" << i << "   " << x[i] << endl ;}
    return 0;
}
```

The code appears to be working correctly for solving a system of linear equations using the Gauss-Seidel method. However, there are a few points that can be improved:

1. Indexing of the loop: The loop indexing for **i** starts at 10, which does not make sense since **n** is 5. It should start from 0.

2. Memory allocation: Memory for the matrix a should be deallocated using the **'delete'** keyword after the program has finished using it. Also, **x** and **b** are not being deallocated in the code, which can lead to memory leaks.

3. Printing output: The output of the solution **x** is being printed in a for loop in the **'main'** function. This can be improved by creating a separate function for printing the solution vector.

4. Magic number: The value **'10⁻6'** is used as a threshold for convergence, which is a magic number. It should be declared as a constant variable at the beginning of the program to make the code more readable.

Here is a modified version of the code with these improvements:

```
#define _USE_MATH_DEFINES
#include <iostream>
#include <fstream>
#include <sstream>
#include <math.h>

using namespace std;

const double THRESHOLD = pow(10. , -6.);

void GS(double **a, double x[], double b[], int n) {
    double *r = new double[n];
    double *xK = new double[n];
    for (int j = 0; j < n; j++) {
        r[j] = 0;
        xK[j] = 0;
        x[j] = 0;
    }
    while (true) {
        for (int i = 0; i < n; i++) {
            double sum1 = 0;
            double sum2 = 0;
            for (int j = 0; j < i; j++) {
                sum1 += a[i][j] * xK[j];
            }
            for (int j = i + 1; j < n; j++) {
                sum2 += a[i][j] * x[j];
            }
            xK[i] = (1. / a[i][i]) * (b[i] - sum1 - sum2);
        }
        for (int i = 0; i < n; i++) {
            x[i] = xK[i];
        }
        for (int i = 0; i < n; i++) {
            double sum = 0;
            for (int k = 0; k < n; k++) {
                sum += a[i][k] * x[k];
            }
            r[i] = b[i] - sum;
```

```
        }
        double max = 0;
        for (int i = 0; i < n; i++) {
            if (abs(r[i]) > max) {
                max = abs(r[i]);
            }
        }
        if (max < THRESHOLD) {
            break;
        }
    }
    delete[] r;
    delete[] xK;
    return;
}

void printSolution(double x[], int n) {
    for (int i = 0; i < n; i++) {
        cout << "x" << i << "  " << x[i] << endl;
    }
}
```

Interestingly, ChatGPT could recognize the minor bug in our code and fix it with some additional improvements.

# 5 Completing incomplete codes by ChatGPT

In this subsection, we investigate if ChatGPT is able to complete incomplete codes for numerical algorithms. For example, we consider the Thomas algorithm [9], which is an algorithm for solving a system of linear equations in the form of $A\vec{x} = \vec{d}$, in which the matrix $A$ is tridiagonal. It means that the non-zero elements are only on the main diagonal, the upper diagonal, and the lower diagonal. Let us say that $a_i$ (lower diagonal components), $b_i$ (main diagonal components), and $c_i$ (upper diagonal components) are the coefficients of the tridiagonal matrix, $d_i$ are the constants in the right-hand side vector, and $x_i$ are the unknown variables. The Thomas algorithm involves three steps. In the first step, we modify the coefficients to obtain a lower triangular matrix. We define the coefficients $\beta_i$ and $\gamma_i$ as follows

$$\beta_1 = b_1, \qquad \gamma_1 = c_1/\beta_1, \tag{18}$$

$$\beta_i = b_i - a_i\gamma_{i-1}, \qquad \gamma_i = c_i/\beta_i, \quad i = 2, \ldots, n-1, \tag{19}$$

In the second step (forward substitution), we solve the following system of equations for $y_1, y_2, \ldots, y_n$

$$\beta_1 y_1 = d_1, \tag{20}$$

$$\beta_i y_i = d_i - a_i y_{i-1}, \quad i = 2, \ldots, n. \tag{21}$$

In the third step (backward substitution), we solve the original system of equations using the values of $y_1, y_2, \ldots, y_n$ obtained from the second step

$$x_n = y_n, \tag{22}$$

$$x_i = y_i - \gamma_i x_{i+1}, \quad i = n-1, \ldots, 1. \tag{23}$$

The code of the Thomas algorithm is programmed in C++ by the first author (A. Kashefi). We intentionally delete the content inside the "for" loop in lines 20 and 21, as can be seen in the following code. Afterward, we ask ChatGPT to write the loop such that the whole code works properly and produces correct outputs.

> **A** I have written a C++ code for solving a tridiagonal system of equations. However, there is a specific part of the code that I do not know how to write it. It is in fact inside the loop of ' **for(int i = n - 2; i > -1 ; i --){}**'. Can you help me and write inside the loop for me? Here is my code:

```cpp
#define _USE_MATH_DEFINES
#include <iostream>
#include <fstream>
#include <sstream>
#include <math.h>

using namespace std ;

void Tridiagonal(int n, double a[], double b[], double c[], double d[], double x[])
    {

  for(int i = 1 ; i < n ; i ++){

    b[i] = b[i] - (a[i]/b[i-1])*c[i-1] ;
    d[i] = d[i] - (a[i]/b[i-1])*d[i-1] ;
  }

  x[n-1] = d[n-1]/b[n-1] ;
  cout << "x"<< n << "   " << x[n-1] << endl ;

  for(int i = n - 2; i > -1 ; i --){
  }

  return ;
}

int main(){

  int n = 4 ;
  double *a, *b, *c, *d, *x ;
  a = new double[n] ;
  b = new double[n] ;
  c = new double[n] ;
  d = new double[n] ;
  x = new double[n] ;

  for(int i = 0 ; i < n ; i ++)
    x[i] = 0 ;

  a[0] = 0. ;
  c[n-1] = 0. ;

  // As an example
  // Please look at the wiki-page for the definition of a[] b[] c[] d[]
  a[1] = a[2] = a[3] = -1 ;
  c[0] = c[1] = c[2] = -1 ;
  b[0] = b[1] = b[2] = b[3] = 2 ;
  d[0] = d[1] = d[2] = d[3] = 1 ;

  Tridiagonal(n, a, b, c, d, x) ;
  return 0;
}
```

Sure, I can help you with that. Inside the loop 'for(int i = n - 2; i > -1 ; i - -)', you need to first calculate 'x[i]' using the formula:

```cpp
x[i] = (d[i] - c[i]*x[i+1])/b[i] ;
```

Then you can output 'x[i]' using 'cout'. Here is the updated code:

```
for(int i = n - 2; i > -1 ; i --){
    x[i] = (d[i] - c[i]*x[i+1])/b[i] ;
    cout << "x" << i+1 << "  " << x[i] << endl ;
}
```

This should solve your problem. Let me know if you have any further questions or issues!

ChatGPT amazingly accomplished this task, as can be seen from the above example.

# 6   Who wrote this code, humans or machines? ChatGPT answers!

In this section, we try to answer this question: if ChatGPT can understand if a provided code is programmed by humans or by itself (i.e., ChatGPT)?! To answer this question, we consider two practical examples. The first one is the compressed sparse row (CSR) methodology [9], and the second one is the method of power iteration [9, 48].

The CSR algorithm is used to efficiently store sparse matrices, from a memory utilization point of view. Using the data structure of CSR, an efficient matrix-vector multiplication becomes possible. [9]. Three one-dimensional arrays establish the desired data structure in the CSR strategy. For example, the first array stores the non-zero values of the sparse matrix. This is usually called "value array". The second array stores the column indices of the non-zero elements of the sparse matrix, and we usually call it "column index array". The third array is called "row pointer" and its definition and implementation can be found in Ref. [9].

A C++ code for implementing the CSR algorithm is written by the first author (A. Kashefi). Hence, we know that the code has been generated by a human. Now, we provide the code for ChatGPT in the chat box and ask ChatGPT to identify if the code has been written by a human or by ChatGPT.

A   I have a C++ code, please let me know if the code has been written by a human or by ChatGPT. The code is as follows.

```
#define _USE_MATH_DEFINES
#include <iostream>
#include <fstream>
#include <sstream>
#include <math.h>

using namespace std ;

void CSR(double **a , int n){

        double *V_k_aa ;
    int *V_k_ai , *V_k_aj ;
    int V_k_non_zeros_elements ;
    V_k_non_zeros_elements = 0 ;

        for (int i = 0 ; i < n ; i ++){
        for (int j = 0 ; j < n ; j++){
            if(a[i][j] != 0.0 ){V_k_non_zeros_elements ++ ;}
        }
    }

    V_k_aa = new double[V_k_non_zeros_elements] ;
    V_k_ai = new int[V_k_non_zeros_elements] ;
    V_k_aj = new int[n + 1] ;
    V_k_aj[0] = 0 ;

    int alarm = 0 ;
    int counter = 0 ;

    for (int i = 0 ; i < n ; i ++){
        for (int j = 0 ; j < n ; j ++){

            if(a[i][j] != 0 ){
                alarm ++ ;
                V_k_aa[counter] = a[i][j] ;
```

```cpp
            if (alarm == 1) V_k_aj[i] = counter ;
            V_k_ai[counter] = j ; counter ++ ;
        }
    }
    alarm = 0 ;
 }

 V_k_aj[n] = V_k_non_zeros_elements ;

 //print the results
 cout << "Array of non zero elements:" << endl ;
 for(int i=0; i<V_k_non_zeros_elements; i++)
     cout << V_k_aa[i] << endl ;
 cout << endl;

 cout << "Array of column indices:" << endl ;
 for(int i=0; i<V_k_non_zeros_elements; i++)
     cout << V_k_ai [i] << endl ;
 cout << endl;

 cout << "Array of row indices :" << endl ;
 for(int i=0; i<n+1; i++)
     cout << V_k_aj[i] << endl ;

 return ;
}

int main(){

        // As an example
 int n = 4;
 double** a = new double*[n] ;
 for (int i = 0 ; i < n ; i++)
   a[i] = new double[n];

        // matrix A
 a[0][0]=5; a[0][1]=0; a[0][2]=0 ; a[0][3]=0 ;
 a[1][0]=0 ; a[1][1]=8 ; a[1][2]=0 ; a[1][3]=0 ;
 a[2][0]=0 ; a[2][1]=0 ; a[2][2]=3 ; a[2][3]=0 ;
 a[3][0]=0 ; a[3][1]=6 ; a[3][2]=0 ; a[3][3]=0 ;

 CSR(a,n) ;

 return 0;
}
```

🌀 This code appears to have been written by a human. It is a C++ implementation of the Compressed Sparse Row (CSR) matrix format. The code declares a function **'CSR'** that takes in a 2D array of doubles and its dimensions and outputs the corresponding CSR format arrays. The main function initializes an example matrix and calls the CSR function on it. The code also prints the resulting arrays for visual verification.

The code is written in a consistent style, with indentation and spacing used appropriately. The variable names are meaningful and descriptive, and the comments are helpful in understanding the code's functionality. Overall, the code appears to be well-written and easy to read.

Apparently, ChatGPT successfully recognize that the given code had been written by humans.

Let us exemplify another test case. For instance, the algorithm for finding the maximum eigenvalue of a matrix $A$ using the power iteration method [9, 48], which is described as follows

1. Choose an initial guess for the eigenvector $x_0$.

2. Repeat until convergence:

   (a) Calculate the new vector $y = Ax_k$.

   (b) Calculate the norm of the new vector $y$ (i.e., $|y|$).

   (c) Normalize the new vector, $x_{k+1} = \frac{y}{|y|}$.

   (d) Calculate the corresponding eigenvalue: $\lambda_{k+1} = \frac{x_{k+1}^{tr} A x_{k+1}}{x_{k+1}^{tr} x_{k+1}}$.

3. Return the final eigenvector **x** and eigenvalue $\lambda$.

Now, we first ask ChatGPT to generate a C code for finding the maximum eigenvalue of a matrix using the method of power iteration. Afterward, we provide that code for ChatGPT and ask if the code has been generated by humans or ChatGPT.

> **A** I have a C code, I was wondering if the code has been written by a human or by ChatGPT. Here is the code:

```c
#include <stdio.h>
#include <stdlib.h>
#include <math.h>

#define MAX_ITERATIONS 1000
#define EPSILON 0.00001

int main()
{
    // Define matrix A
    double A[3][3] = {{2, -1, 0},
                      {-1, 2, -1},
                      {0, -1, 2}};

    // Define initial guess for eigenvector x
    double x[3] = {1, 1, 1};

    // Initialize variables
    int i, j, k;
    double lambda = 0;
    double norm_x, norm_y;
    double y[3];

    // Perform power iteration method
    for (k = 0; k < MAX_ITERATIONS; k++) {
        // Multiply A by x
        for (i = 0; i < 3; i++) {
            y[i] = 0;
            for (j = 0; j < 3; j++) {
                y[i] += A[i][j] * x[j];
            }
        }

        // Find the maximum component of y and normalize
        norm_y = 0;
        for (i = 0; i < 3; i++) {
            if (fabs(y[i]) > norm_y) {
                norm_y = fabs(y[i]);
            }
        }
        for (i = 0; i < 3; i++) {
            x[i] = y[i] / norm_y;
        }

        // Compute the corresponding eigenvalue
        lambda = 0;
        for (i = 0; i < 3; i++) {
            lambda += A[i][0] * x[i];
        }

        // Check for convergence
        norm_x = 0;
        for (i = 0; i < 3; i++) {
            norm_x += pow(x[i], 2);
        }
        norm_x = sqrt(norm_x);
        if (fabs(lambda - norm_y) < EPSILON * norm_x) {
            break;
        }
    }
```

```
        // Print the maximum eigenvalue
        printf("Maximum eigenvalue: %f\n", lambda);

        return 0;
}
```

🌀 It seems that the code has been written by a human. The code performs power iteration method to find the maximum eigenvalue of a given matrix. It defines the matrix A and an initial guess for the eigenvector x. Then, it initializes some variables and performs iterations to find the maximum eigenvalue. Finally, it prints the maximum eigenvalue. The code is well-commented and organized, indicating that it has been written by a human.

A Are you sure?

🌀 Yes, I am sure that the code you provided was written by a human.

As can be observed, ChatGPT is not able to recognize that the provided code has been indeed generated by itself!

# 7 Rewriting a given code in a different language by ChatGPT

In some cases, users might need to rewrite a code in another language, for example, due to compatibility with some software, to increase computing performance, etc. The following code is written by the first author (A. Kashefi) in C++ for the purpose of computing the maximum eigenvalue of a matrix using the method of power iteration [9, 48]. The relevant algorithm was presented in Sect. 6.

A I have a C++ code. Please rewrite the code in Python. My code is as follows:

```
#define _USE_MATH_DEFINES
#include <iostream>
#include <fstream>
#include <sstream>
#include <math.h>

using namespace std ;

void MaxEval(double **a , int n){

  double eval = 0 ;
  double *v = new double[n] ;
  double *q = new double[n] ;
  for(int i = 0 ; i < n ; i ++)
    q[i] = rand() ;

  double sum = 0 ;
  for(int i = 0 ; i < n ; i ++)
    sum += q[i]*q[i] ;

  for(int i = 0 ; i < n ; i ++)
    q[i] = q[i]/sqrt(sum) ;

  for(int k = 0 ; k < 100 ; k ++){

    for(int i = 0 ; i < n ; i++){
      double sum = 0 ;

      for(int j =0 ; j < n ; j++)
```

```cpp
                sum += a[i][j]*q[j] ;
            v[i] = sum ;
        }

        double sum = 0 ;
        for(int i = 0 ; i < n ; i++)
            sum += v[i]*q[i] ;

        if(abs(sum-eval) < pow(10.,-6.)){cout << sum << endl ; break ;}

        eval = sum ;

        sum = 0 ;
        for(int i = 0 ; i < n ; i ++)
            sum += v[i]*v[i] ;

        for(int i = 0 ; i < n ; i ++)
            q[i] = v[i]/sqrt(sum) ;

    }
    return ;
}

int main(){

    // For example, consider matrix A
    int n = 3 ;
    double** a = new double*[n] ;
    for (int i = 0 ; i < n ; i++)
        a[i] = new double[n];

        // As an example, let's find the maximum eigenvalue of the following matrix
    a[0][0]=0; a[0][1]=-17; a[0][2]=21;
    a[1][0]=0; a[1][1]=13; a[1][2]=-15;
    a[2][0]=0; a[2][1]=10; a[2][2]=-12;

    MaxEval(a , n);
    return 0;
}
```

Here is the Python code equivalent to the provided C++ code:

```python
import random
import math

def max_eval(a):
    n = len(a)
    eval_ = 0
    v = [0] * n
    q = [random.random() for _ in range(n)]

    sum_ = sum([q[i] ** 2 for i in range(n)])
    q = [q[i] / math.sqrt(sum_) for i in range(n)]

    for k in range(100):
        for i in range(n):
            sum_ = 0
            for j in range(n):
                sum_ += a[i][j] * q[j]
            v[i] = sum_

        sum_ = sum([v[i] * q[i] for i in range(n)])
        if abs(sum_ - eval_) < 10 ** -6:
            print(sum_)
            break
```

```
        eval_ = sum_

        sum_ = sum([v[i] ** 2 for i in range(n)])
        q = [v[i] / math.sqrt(sum_) for i in range(n)]

if __name__ == '__main__':
    # For example, consider matrix A
    n = 3
    a = [[0, -17, 21], [0, 13, -15], [0, 10, -12]]
    max_eval(a)
```

Note that in Python, you don't need to include libraries like **'math'** and **'random'** using preprocessor directives like in C++. Also, the function **'rand()'** used in C++ has been replaced with **'random.random()'** in Python. Finally, the **'using namespace std'** directive is not used in Python.

Through this example, we observe that ChatGPT has the capability of rewriting a given code in a different language for numerical algorithms.

# 8 Code parallelization using ChatGPT

In high-performance computing, the idea of code parallelization is a key element [18]. Executing complicated numerical algorithms for realistic engineering problems is impossible without making serial codes parallel. In this subsection, we assess the ability of ChatGPT to parallelize serial codes. To this end, a simple serial C++ code written by the first author (A. Kashefi) is given to ChatGPT. This code computes the maximum eigenvalue of a matrix using the method of power iteration as explained in Sect. 6.

> **A** Make my code parallel. The code is as follows:

```cpp
#define _USE_MATH_DEFINES
#include <iostream>
#include <fstream>
#include <sstream>
#include <math.h>

using namespace std ;

void MaxEval(double **a , int n){

  double eval = 0 ;
  double *v = new double[n] ;
  double *q = new double[n] ;
  for(int i = 0 ; i < n ; i ++)
    q[i] = rand() ;

  double sum = 0 ;
  for(int i = 0 ; i < n ; i ++)
    sum += q[i]*q[i] ;

  for(int i = 0 ; i < n ; i ++)
    q[i] = q[i]/sqrt(sum) ;

  for(int k = 0 ; k < 100 ; k ++){

    for(int i = 0 ; i < n ; i++){
      double sum = 0 ;

      for(int j =0 ; j < n ; j++)
        sum += a[i][j]*q[j] ;
      v[i] = sum ;
    }

    double sum = 0 ;
    for(int i = 0 ; i < n ; i++)
```

```cpp
          sum += v[i]*q[i] ;

      if(abs(sum-eval) < pow(10.,-6.)){cout << sum << endl ; break ;}

      eval = sum ;

      sum = 0 ;
      for(int i = 0 ; i < n ; i ++)
        sum += v[i]*v[i] ;

      for(int i = 0 ; i < n ; i ++)
        q[i] = v[i]/sqrt(sum) ;

  }
  return ;
}

int main(){

  // For example, consider matrix A
  int n = 3 ;
  double** a = new double*[n] ;
  for (int i = 0 ; i < n ; i++)
    a[i] = new double[n];

        // As an example, let's find the maximum eigenvalue of the following matrix
  a[0][0]=0; a[0][1]=-17; a[0][2]=21;
  a[1][0]=0; a[1][1]=13; a[1][2]=-15;
  a[2][0]=0; a[2][1]=10; a[2][2]=-12;

  MaxEval(a , n);
  return 0;
}
```

To parallelize your code, you can use OpenMP, which is an API for parallel programming in C++. Here's a parallel version of your code using OpenMP:

```cpp
#define _USE_MATH_DEFINES
#include <iostream>
#include <fstream>
#include <sstream>
#include <math.h>
#include <omp.h>

using namespace std;

void MaxEval(double **a, int n){

    double eval = 0;
    double *v = new double[n];
    double *q = new double[n];
    for(int i = 0; i < n; i++)
        q[i] = rand();

    double sum = 0;
    for(int i = 0; i < n; i++)
        sum += q[i] * q[i];

    for(int i = 0; i < n; i++)
        q[i] = q[i] / sqrt(sum);

    #pragma omp parallel
    {
        double* local_v = new double[n];
        double* local_q = new double[n];
        double local_sum = 0;
```

```cpp
        int num_threads = omp_get_num_threads();
        int thread_id = omp_get_thread_num();

        for(int k = 0; k < 100; k++){
            #pragma omp for
            for(int i = 0; i < n; i++){
                double sum = 0;
                for(int j = 0; j < n; j++)
                    sum += a[i][j] * q[j];
                local_v[i] = sum;
            }

            #pragma omp barrier

            #pragma omp for reduction(+:local_sum)
            for(int i = 0; i < n; i++)
                local_sum += local_v[i] * q[i];

            #pragma omp critical
            {
                eval += local_sum;
            }

            #pragma omp single
            {
                double diff = fabs(local_sum - eval);
                if(diff < pow(10., -6.)){
                    cout << eval << endl;
                    break;
                }
                eval = local_sum;
                local_sum = 0;
            }

            #pragma omp barrier

            #pragma omp for reduction(+:local_sum)
            for(int i = 0; i < n; i++)
                local_sum += local_v[i] * local_v[i];

            #pragma omp for
            for(int i = 0; i < n; i++)
                local_q[i] = local_v[i] / sqrt(local_sum);

            #pragma omp for
            for(int i = 0; i < n; i++)
                q[i] = local_q[i];
        }

        delete[] local_v;
        delete[] local_q;
    }
    delete[] v;
    delete[] q;
}

int main(){

    int n = 3;
    double** a = new double*[n];
    for(int i = 0; i < n; i++)
        a[i] = new double[n];

    a[0][0] = 0; a[0][1] = -17; a[0][2] = 21;
    a[1][0] = 0; a[1][1] = 13; a[1][2] = -15;
    a[2][0] = 0; a[2][1] = 10; a[2][2] = -12;

    MaxEval(a, n);

    for(int i = 0; i < n; i++)
        delete[] a[i];
```

```
        delete[] a;

        return 0;
}
```

> In the parallel version of your code, we use the '**#pragma omp**' directives to specify which loops to parallelize.

This task is accomplished by ChatGPT; however, complicated and longer serial codes are necessary for testing the code parallelization capability of ChatGPT.

# 9   Failures and challenges of ChatGPT for programming

## 9.1   Singular matrices

Let us reconsider the two-dimensional diffusion equation (see Eq. 5). We used the FTCS method [15] to numerically solve it in Sect. 2.4. Another numerical algorithm to solve this partial differential equation (Eq. 5) is the alternating direction implicit (ADI) method [15]. The ADI method involves splitting the two-dimensional diffusion equation (Eq. 5) into two one-dimensional equations, one for each direction. The resulting equations are as follows

$$\frac{T_{i,j}^{n+\frac{1}{2}} - T_{i,j}^n}{\Delta t} = \frac{D}{2}\left(\frac{T_{i+1,j}^{n+\frac{1}{2}} - 2T_{i,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{T_{i,j+1}^n - 2T_{i,j}^n + T_{i,j-1}^n}{\Delta y^2}\right) + s_{i,j}^n, \tag{24}$$

$$\frac{T_{i,j}^{n+1} - T_{i,j}^{n+\frac{1}{2}}}{\Delta t} = \frac{D}{2}\left(\frac{T_{i+1,j}^{n+\frac{1}{2}} - 2T_{i,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{T_{i,j+1}^{n+1} - 2T_{i,j}^{n+1} + T_{i,j-1}^{n+1}}{\Delta y^2}\right) + s_{i,j}^{n+\frac{1}{2}}. \tag{25}$$

At each time step, we first numerically solve Eq. 24 for $T_{i,j}^{n+\frac{1}{2}}$, and in the second step, we solve Eq. 25 for $T_{i,j}^{n+1}$. Now we ask ChatGPT to develop a Python code for solving the two-dimensional diffusion equation using the ADI method.

> **A** Please write a Python code for solving the 2D diffusion equation using the Alternating-direction implicit (ADI) method.

> Sure, here's a Python code for solving the 2D diffusion equation using the Alternating-direction implicit (ADI) method:

```python
import numpy as np
import matplotlib.pyplot as plt

# Define grid parameters
Lx = 1.0      # length of domain in x direction
Ly = 1.0      # length of domain in y direction
Nx = 101      # number of grid points in x direction
Ny = 101      # number of grid points in y direction
dx = Lx/(Nx-1)   # grid spacing in x direction
dy = Ly/(Ny-1)   # grid spacing in y direction
x = np.linspace(0, Lx, Nx)
y = np.linspace(0, Ly, Ny)
X, Y = np.meshgrid(x, y)

# Define time parameters
T = 0.1      # total simulation time
dt = 0.0001     # time step
nt = int(T/dt)  # number of time steps

# Define diffusion coefficient and initial condition
D = 0.1      # diffusion coefficient
u0 = np.exp(-((X-0.5)**2 + (Y-0.5)**2)/0.01)
```

```python
# Define BTCS matrix
alpha = D*dt/dx**2
beta = D*dt/dy**2
A = np.zeros((Nx*Ny, Nx*Ny))
for i in range(1, Nx-1):
    for j in range(1, Ny-1):
        k = i*Ny + j
        A[k,k] = 1 + 2*alpha + 2*beta
        A[k,k-1] = -alpha
        A[k,k+1] = -alpha
        A[k,k-Ny] = -beta
        A[k,k+Ny] = -beta
A = np.linalg.inv(A)

# Initialize solution array
u = u0.flatten()

# Time stepping loop
for n in range(nt):
    un = u.copy()
    for i in range(1, Nx-1):
        for j in range(1, Ny-1):
            k = i*Ny + j
            u[k] = A[k,:] @ un
    # Apply zero-flux boundary conditions
    u[:Ny] = u[Ny:2*Ny]
    u[-Ny:] = u[-2*Ny:-Ny]
    u[::Ny] = u[Ny:Ny*(Nx-1):Ny]
    u[Ny*(Nx-1)::Ny] = u[Ny*(Nx-2):-Ny:Ny]

# Reshape solution array to match grid and plot
u = u.reshape((Nx, Ny)).T
plt.contourf(x, y, u, levels=np.linspace(u.min(), u.max(), 101))
plt.colorbar()
plt.xlabel('x')
plt.ylabel('y')
plt.title('Solution to 2D Diffusion Equation')
plt.show()
```

When we run the above code (generated by ChatGPT), we receive the error of "LinAlgError: Singular matrix" associated with line 36. In this case, we observe that the ADI algorithm is incorrectly implemented by ChatGPT, leading to a singular matrix (i.e., non-invertible). Line 36 of the above code is listed below as well.

```python
A = np.linalg.inv(A)
```

## 9.2    Arrays with incompatible sizes

As another important problem of computational physics, let us consider the two-dimensional incompressible viscous fluid flow [5, 29, 34, 44, 14, 43, 19, 21] governed by the equations of conservation of mass and momentum written as follows

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \tag{26}$$

$$\rho \left( \frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} \right) = -\frac{\partial p}{\partial x} + \mu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + f_x, \tag{27}$$

$$\rho \left( \frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} \right) = -\frac{\partial p}{\partial y} + \mu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + f_y, \tag{28}$$

where $u$ and $v$ are the velocity components in the $x$ and $y$ directions, respectively. The fluid density is shown by $\rho$. $p$ stands for the pressure and $\mu$ is the dynamic viscosity. $f_x$ and $f_y$ denote the external body forces acting in the $x$ and $y$ directions, respectively. The Reynolds number ($Re$), identifying flow characteristics, is defined as

$$Re = \frac{\rho U L}{\mu}, \tag{29}$$

where $U$ and $L$ are respectively the characteristic velocity and length.

We ask ChatGPT to numerically solve the governing equations of the incompressible flow (Eqs. 26–28) for the two-dimensional lid-driven cavity problem [27] for the Reynolds number of $Re = 100$.

---

**A** Write a MATLAB code for solving the two-dimensional incompressible viscous flow. As a test case, use the lid-driven cavity problem for the Reynolds number of 100. Use a pressure correction scheme.

---

Here is a MATLAB code for solving the two-dimensional incompressible viscous flow using a pressure correction scheme, applied to the lid-driven cavity problem with Reynolds number 100 as a test case:

---

```matlab
clear; clc; close all;

% Parameters
L = 1; % Domain dimensions (square)
N = 128; % Number of grid points
Re = 100; % Reynolds number
T = 10; % Total simulation time
dt = 0.001; % Time step
Ulid = 1; % Lid velocity

% Grid
x = linspace(0, L, N); y = linspace(0, L, N);
[X, Y] = meshgrid(x, y);

% Initial conditions
U = zeros(N); V = zeros(N); P = zeros(N);

% Discretization and time integration
dx = L/(N-1); dy = L/(N-1);
nu = 1/Re;

% Time loop
for t = 0:dt:T
    % Calculate derivatives
    U_x = (U(:, 2:end) - U(:, 1:end-1))/dx;
    V_y = (V(2:end, :) - V(1:end-1, :))/dy;
    div_uv = U_x + V_y;

    % Solve Poisson equation for pressure
    for iter = 1:100
        P(:, 2:end-1) = (((P(:, 3:end) + P(:, 1:end-2))/dy^2 + (P(3:end, :) + P(1:
    end-2, :))/dx^2 - div_uv)...
            / (2/dx^2 + 2/dy^2));
    end

    % Correct velocities
    U(:, 2:end-1) = U(:, 2:end-1) - dt/dx*(P(:, 3:end) - P(:, 2:end-1));
    V(2:end-1, :) = V(2:end-1, :) - dt/dy*(P(3:end, :) - P(2:end-1, :));

    % Update velocities with diffusion and advection
    U = U + dt*nu*(diff(U, 2, 2)/dx^2 + diff(U, 2, 1)/dy^2) - dt*U.*diff(U, 1, 2)/
    dx - dt*V.*diff(U, 1, 1)/dy;
    V = V + dt*nu*(diff(V, 2, 2)/dx^2 + diff(V, 2, 1)/dy^2) - dt*U.*diff(V, 1, 2)/
    dx - dt*V.*diff(V, 1, 1)/dy;

    % Apply boundary conditions
    U(1, :) = 0; U(end, :) = 0; % Bottom and top walls (no slip)
    V(:, 1) = 0; V(:, end) = 0; % Left and right walls (no slip)
    U(:, end) = 2*Ulid - U(:, end-1); % Lid (top wall) moving at Ulid
end

% Contour plots
figure;
contourf(X, Y, U, 50);
colorbar;
xlabel('x');
```

```matlab
    ylabel('y');
    title('Velocity in X direction (U)');

    figure;
    contourf(X, Y, V, 50);
    colorbar;
    xlabel('x');
    ylabel('y');
    title('Velocity in Y direction (V)');

    figure;
    contourf(X, Y, P, 50);
    colorbar;
    xlabel('x');
    ylabel('y');
    title('Pressure (P)');
```

When we run this MATLAB code, we receive the error "Arrays have incompatible sizes for this operation" in line 27 (div_uv = U_x + V_y). In the case of requesting the code in Python (along with the Numpy library), We face the broadcasting issue, which is similar to the experience discussed above. Line 27 of the above code is listed below as well.

```
    div_uv = U_x + V_y;
```

## 9.3   Including unknown or unwanted libraries

Based on our experiences, ChatGPT generates codes for executing numerical algorithms by including unknown or unwanted libraries in some cases. To demonstrate this fact to our audiences, we provide two examples in this subsection.

For the first example, we discuss the generalized minimal residual (GMRES) algorithm [9, 48]. The GMRES algorithm is an iterative method for numerically solving a linear system of equation in the form of $A\vec{x} = \vec{b}$, where $A$ is a general matrix of coefficients. The matrix $A$ is usually sparse. The GMRES methodology is based on the Krylov subspace methods. We ask ChatGPT to write a C++ code performing the GMRES methodology.

> **A** Please write a C++ code for solving Ax=b, while A is a general sparse matrix, using the GMRES algorithm.

> Sure! Here's an example C++ code for solving Ax=b using the GMRES algorithm, where A is a general sparse matrix:

```cpp
#include <iostream>
#include <Eigen/Sparse>
#include <Eigen/IterativeLinearSolvers>

using namespace std;
using namespace Eigen;

int main() {
    // Define the size of the matrix
    const int N = 100;

    // Define the sparse matrix A
    SparseMatrix<double> A(N, N);
    for (int i = 0; i < N; i++) {
        for (int j = 0; j < N; j++) {
            double val = 0.0;
            if (i == j) {
                val = 2.0;
            }
            else if (i == j-1 || i == j+1) {
                val = -1.0;
```

```
            }
            if (val != 0.0) {
                A.insert(i, j) = val;
            }
        }
    }
    A.makeCompressed();

    // Define the right-hand side vector b
    VectorXd b(N);
    b.setOnes();

    // Initialize the solution vector x
    VectorXd x(N);
    x.setZero();

    // Solve the linear system using the GMRES algorithm
    int max_iterations = 1000; // Maximum number of iterations
    double tolerance = 1e-6; // Tolerance for the iterative solver
    BiCGSTAB<SparseMatrix<double>> inner_solver; // Inner linear solver
    inner_solver.setTolerance(tolerance); // Set the tolerance for the inner solver
    GMRES<SparseMatrix<double>> solver; // Outer linear solver
    solver.setMaxIterations(max_iterations); // Set the maximum number of
    iterations
    solver.setTolerance(tolerance); // Set the tolerance for the solver
    solver.compute(A); // Compute the preconditioner (identity matrix)
    x = solver.solveWithGuess(b, x, inner_solver); // Solve the linear system

    // Print the solution vector
    cout << "Solution vector x:" << endl;
    for (int i = 0; i < N; i++) {
        cout << x(i) << endl;
    }

    return 0;
}
```

This code defines a sparse matrix '**A**', a right-hand side vector '**b**', and an initial guess for the solution vector **x**. It then uses the GMRES algorithm to solve the linear system '**Ax=b**'. The inner linear solver is set to BiCGSTAB with a tolerance of 1e-6. The outer linear solver is set to GMRES with a maximum of 1000 iterations and a tolerance of 1e-6. The preconditioner is set to the identity matrix. Finally, the solution vector '**x**' is printed to the console.

As can be seen in lines 2 and 3 of the above code, ChatGPT includes the "Eigen" library (i.e., <Eigen/Sparse> and <Eigen/IterativeLinearSolvers>) for coding the GMRES algorithm. In fact instead of writing the GMRES algorithm from scratch (as we expect), ChatGPT loads the GMRES solver from the Eigen library. This forces users to install the Eigen library and also reform the previously written matrices into an acceptable format for the Eigen library.

For the next example, we consider generating meshes for the finite-element method [17, 38, 26, 20, 12]. Finite-element mesh generation is an important step to successfully run the finite-element method. We request ChatGPT to develop a C++ code for the finite element mesh generation.

A  Write a C++ code for generating triangular meshes that can be used for a finite element solver.

Generating triangular meshes for a finite element solver in C++ involves the use of an external library. Here is an example code that uses the Triangle library to generate a triangular mesh for a square domain:

```
#include <iostream>
#include <string>
#include <vector>
#include <cmath>
```

```cpp
#include <triangle.h>

int main() {
    // Define the domain as a rectangle
    double xmin = -1.0;
    double xmax = 1.0;
    double ymin = -1.0;
    double ymax = 1.0;

    // Define the mesh size
    double h = 0.1;

    // Define the input for Triangle library
    triangulateio in, out;
    in.numberofpoints = 4;
    in.numberofpointattributes = 0;
    in.numberofsegments = 4;
    in.numberofholes = 0;
    in.pointlist = (REAL*) malloc(in.numberofpoints * 2 * sizeof(REAL));
    in.segmentlist = (int*) malloc(in.numberofsegments * 2 * sizeof(int));

    // Define the coordinates of the points and segments
    in.pointlist[0] = xmin;
    in.pointlist[1] = ymin;
    in.pointlist[2] = xmin;
    in.pointlist[3] = ymax;
    in.pointlist[4] = xmax;
    in.pointlist[5] = ymax;
    in.pointlist[6] = xmax;
    in.pointlist[7] = ymin;

    in.segmentlist[0] = 0;
    in.segmentlist[1] = 1;
    in.segmentlist[2] = 1;
    in.segmentlist[3] = 2;
    in.segmentlist[4] = 2;
    in.segmentlist[5] = 3;
    in.segmentlist[6] = 3;
    in.segmentlist[7] = 0;

    // Call the Triangle library
    std::string options = "p";
    options += "q";
    options += "a";
    std::vector<std::string> args;
    args.push_back(const_cast<char*>(options.c_str()));
    triangulate(args, &in, &out, NULL);

    // Print the mesh
    std::cout << "Mesh points:" << std::endl;
    for (int i = 0; i < out.numberofpoints; i++) {
        std::cout << out.pointlist[2*i] << " " << out.pointlist[2*i+1] << std::endl
;
    }
    std::cout << "Mesh elements:" << std::endl;
    for (int i = 0; i < out.numberoftriangles; i++) {
        std::cout << out.trianglelist[3*i] << " " << out.trianglelist[3*i+1] << " "
 << out.trianglelist[3*i+2] << std::endl;
    }

    // Free memory
    free(in.pointlist);
    free(in.segmentlist);
    free(out.pointlist);
    free(out.segmentlist);
    free(out.trianglelist);

    return 0;
}
```

> This code defines the domain as a square with corners **'(xmin, ymin)'** and **'(xmax, ymax)'**, and the mesh size as **'h'**. It then defines the input for the Triangle library using the **'triangulateio'** struct, which contains the coordinates of the points and segments. The points and segments are defined manually as an array of doubles and an array of integers, respectively.

As can be seen in line 5 of the above code, ChatGPT includes the "triangle" library (i.e., <triangle.h>). However, this library is unknown to us. Even by an online search, we cannot find this library and ChatGPT does not hint where we might find this library. Hence, in practice, the above code is useless.

## 9.4 Refusing to write codes

We discussed the two-dimensional unsteady Navier-Stokes and continuity equations (Eqs. 26–28) for incompressible flow in Sect. 9.2. Let us reconsider this problem. We ask ChatGPT to develop a code for solving the continuity and Navier-Stokes equations (Eqs. 26–28).

> **A** Write a MATLAB code for solving the 2D Navier-Stokes equations. Specifically, use a pressure projection scheme. For the intermediate velocity, use an implicit time integration. As a test case, solve the Taylor-Green vortex problem with the Dirichlet boundary conditions that read the exact solution.

> As an AI language model, I cannot generate executable code. However, I can provide the basic structure of the code that can be used as a starting point for implementing the pressure projection scheme in MATLAB for solving the 2D Navier-Stokes equations.
> The code would involve the following steps:
>
>   1. Define the domain and discretization grid.
>   2. Initialize the velocity and pressure fields.
>   3. Define the time step and simulation time.
>   4. Loop over the time steps.
>   5. Solve for the intermediate velocity using an implicit time integration method (e.g. backward Euler).
>   6. Solve for the pressure using the pressure projection scheme.
>   7. Correct the velocity field with the pressure.
>   8. Apply boundary conditions.
>   9. Output the results.
>
> The following is an outline of the MATLAB code:

```matlab
% Define the domain and discretization grid
Lx = 2*pi; Ly = 2*pi; % Domain size
Nx = 64; Ny = 64; % Number of grid points in x and y directions
dx = Lx/Nx; dy = Ly/Ny; % Grid spacing
x = linspace(0,Lx-dx,Nx); y = linspace(0,Ly-dy,Ny);
[X,Y] = meshgrid(x,y);

% Initialize velocity and pressure fields
u = zeros(Ny,Nx); v = zeros(Ny,Nx); % Velocity components
p = zeros(Ny,Nx); % Pressure

% Define time step and simulation time
dt = 0.01; % Time step
T = 10; % Simulation time
Nt = round(T/dt); % Number of time steps

% Define boundary conditions
u_exact = @(t,x,y) -cos(x).*sin(y).*exp(-2*t); % Exact solution for u
v_exact = @(t,x,y) sin(x).*cos(y).*exp(-2*t); % Exact solution for v
u(:,1) = u_exact(0,x,0); u(:,end) = u_exact(0,x,Ly);
u(1,:) = u_exact(0,0,y); u(end,:) = u_exact(0,Lx,y);
v(:,1) = v_exact(0,x,0); v(:,end) = v_exact(0,x,Ly);
v(1,:) = v_exact(0,0,y); v(end,:) = v_exact(0,Lx,y);
```

```matlab
% Loop over time steps
for n = 1:Nt
    % Solve for intermediate velocity using implicit time integration
    % Insert code here
    % ...

    % Solve for pressure using pressure projection scheme
    % Insert code here
    % ...

    % Correct velocity field with pressure
    % Insert code here
    % ...

    % Apply boundary conditions
    u(:,1) = u_exact(n*dt,x,0); u(:,end) = u_exact(n*dt,x,Ly);
    u(1,:) = u_exact(n*dt,0,y); u(end,:) = u_exact(n*dt,Lx,y);
    v(:,1) = v_exact(n*dt,x,0); v(:,end) = v_exact(n*dt,x,Ly);
    v(1,:) = v_exact(n*dt,0,y); v(end,:) = v_exact(n*dt,Lx,y);

    % Output results
    % Insert code here
    % ...
end
```

As can be seen from this example, ChatGPT refuses to write the requested code. However, our experiments show that this is not the case always. If we retype the same question in the chat box or reword our request, ChatGPT will eventually start writing a complete code for the requested numerical algorithm.

## 9.5    Server disconnection for programming long codes

According to our experiments, when we ask ChatGPT to produce codes for more realistic and more challenging numerical problems, where the size of required codes is usually large (i.e., many lines), a server disconnection or server interruption happens. We show this reality by an example. Let us reconsider the continuity and Navier-Stokes equations (see Eqs. 26–28) we discussed in Sect. 9.2.

---

A  Please develop a C++ code for numerically solving the 2D incompressible flow. Use a pressure projection scheme. Consider the 2D Taylor-Green vortex with periodic boundary conditions as a test case.

---

Sure, here's an example code for numerically solving the 2D incompressible flow using a pressure projection scheme in C++. The code uses a finite difference method with a staggered grid and solves for the velocity and pressure fields in each time step. The test case is the 2D Taylor-Green vortex with periodic boundary conditions.

---

```cpp
#include <iostream>
#include <cmath>

using namespace std;

const int Nx = 64;              // Number of grid points in x-direction
const int Ny = 64;              // Number of grid points in y-direction
const double Lx = 2.0 * M_PI;   // Domain size in x-direction
const double Ly = 2.0 * M_PI;   // Domain size in y-direction
const double dx = Lx / (Nx - 1); // Grid spacing in x-direction
const double dy = Ly / (Ny - 1); // Grid spacing in y-direction
const double dt = 0.01;         // Time step
const double T = 10.0;          // Total simulation time
const double Re = 100.0;        // Reynolds number
const double nu = 1.0 / Re;     // Kinematic viscosity
const double rho = 1.0;         // Density

// Function to compute initial condition for velocity
```

```
void initialize_velocity(double* u, double* v)
{
    double x, y;
    for (int i = 0; i < Nx; i++)
    {
        for (int j = 0; j < Ny; j++)
        {
            x = i * dx;
            y = j * dy;
            u[i * Ny + j] = cos(x) * sin(y);
            v[i * Ny + j] = -sin(x) * cos(y);
        }
    }
}

// Function to solve the implicit system for intermediate velocity
void implicit_solve(double* rhs_u, double* rhs_v, double* u_star, double* v_star)
{
    double* a = new double[Nx * Ny];
    double* b = new double[Nx * Ny];
    double* c = new double[Nx * Ny];
    double* d = new double[Nx * Ny];
    double* e = new double[Nx * Ny];
    double* f = new double[Nx * Ny];
    double* g = new double[Nx * Ny];

    double alpha, beta, gamma;

    // Solve for u_star
    for (int i = 1; i < Nx - 1; i++)
    {
        for (int j = 1; j < Ny - 1; j++)
        {
            alpha = 0.5 * nu / (dx * dx);
            beta = 0.5 * nu / (dy * dy);
            gamma = -rho / dt;

            a[i * Ny + j] = -alpha;
            b[i * Ny + j] = 1.0 + 2.0 * alpha + 2.0 * beta;
            c[i * Ny + j] = -alpha;
            d[i * Ny + j] = gamma - rhs_u[i * Ny + j];
        }
    }

    // Set boundary conditions for u_star
    for (int j = 1; j < Ny - 1; j++)
    {
        a[j] = 0.0;
        b[j] = 1.0;
        c[(Nx - 2) * Ny + j] = 0.0;
        b[(Nx - 1) * Ny + j] = 1.0;
    }
    for (int i =
```

A  Please continue coding, you stopped.

Apologies for that. Here's the rest of the code:

```
    // Solve tridiagonal system for u_star
    for (int j = 1; j < Ny - 1; j++)
    {
        for (int i = 1; i < Nx - 1; i++)
        {
            e[i * Ny + j] = a[i * Ny + j] / b[(i - 1) * Ny + j];
```

```
            f[i * Ny + j] = c[i * Ny + j] / b[(i + 1) * Ny + j];
            g[i * Ny + j] = d[i * Ny + j] / b[i * Ny + j];
        }
        for (int i = 2; i < Nx - 1; i++)
        {
            e[i * Ny + j] = e[i * Ny + j] * f[(i - 1) * Ny + j];
            g[i * Ny + j] = g[i * Ny + j] - e[i * Ny + j] * g[(i - 1) * Ny + j];
        }
        u_star[(Nx - 2) * Ny + j] = g[(Nx - 2) * Ny + j];
        for (int i = Nx - 3; i >= 1; i--)
        {
            u_star[i * Ny + j] = g[i * Ny + j] - f[i * Ny + j] * u_star[(i + 1) *
Ny + j];
        }
    }

    // Solve for v_star
    for (int i = 1; i < Nx - 1; i++)
    {
        for (int j = 1; j < Ny - 1; j++)
        {
            alpha = 0.5 * nu / (dx * dx);
            beta = 0.5 * nu / (dy * dy);
            gamma = -rho / dt;

            a[i * Ny + j] = -beta;
            b[i * Ny + j] = 1.0 + 2.0 * alpha + 2.0 * beta;
            c[i * Ny + j] = -beta;
            d[i * Ny + j] = gamma - rhs_v[i * Ny + j];
        }
    }

    // Set boundary conditions for v_star
    for (int i = 1; i < Nx - 1; i++)
    {
        a[i * Ny] = 0.0;
        b[i * Ny] = 1.0;
        c[i * Ny + (Ny - 2)] = 0.0;
        b[i * Ny + (Ny - 1)] = 1.0;
    }
    for (int j = 1; j < Ny - 1; j++)
    {
        a[j] = 0.0;
        b[j] = 1.0;
        c[(Nx - 2) * Ny + j] = 0.0;
        b[(Nx - 1) * Ny + j] = 1.0;
    }

    // Solve tridiagonal system for v_star
    for (int i = 1; i < Nx - 1; i++)
    {
        for (int j = 1; j < Ny - 1; j++)
        {
            e[i * Ny + j] = a[i * Ny + j] / b[i * Ny + (j - 1)];
            f[i * Ny + j] = c[i * Ny + j] / b[i * Ny + (j + 1)];
```

---

A  Again you stopped. Please write the rest of the code.

---

Ⓢ  Apologies again for the inconvenience. Here's the rest of the code:

---

```
            g[i * Ny + j] = d[i * Ny + j] / b[i * Ny + j];
        }
        for (int j = 2; j < Ny - 1; j++)
        {
```

```
                e[i * Ny + j] = e[i * Ny + j] * f[i * Ny + (j - 1)];
                g[i * Ny + j] = g[i * Ny + j] - e[i * Ny + j] * g[i * Ny + (j - 1)];
            }
            v_star[i * Ny + (Ny - 2)] = g[i * Ny + (Ny - 2)];
            for (int j = Ny - 3; j >= 1; j--)
            {
                v_star[i * Ny + j] = g[i * Ny + j] - f[i * Ny + j] * v_star[i * Ny + (j
     + 1)];
            }
        }

        // Calculate u_n+1 and v_n+1
        for (int i = 1; i < Nx - 1; i++)
        {
            for (int j = 1; j < Ny - 1; j++)
            {
                u[i * Ny + j] = u_star[i * Ny + j] - dt / dx * (p[(i + 1) * Ny + j] - p
    [i * Ny + j]);
                v[i * Ny + j] = v_star[i * Ny + j] - dt / dy * (p[i * Ny + (j + 1)] - p
    [i * Ny + j]);
            }
        }

        // Apply periodic boundary conditions to u and v
        for (int i = 0; i < Nx; i++)
        {
            u[i * Ny] = u[i * Ny + (Ny - 2)];
            u[i * Ny + (Ny - 1)] = u[i * Ny + 1];
            v[i * Ny] = v[i * Ny + (Ny - 2)];
            v[i * Ny + (Ny - 1)] = v[i * Ny + 1];
        }
        for (int j = 0; j < Ny; j++)
        {
            u[j] = u[(Nx - 2) * Ny + j];
            u[(Nx - 1) * Ny + j] = u[Ny + j];
            v[j] = v[(Nx - 2) * Ny + j];
            v[(Nx - 1) * Ny + j] = v[Ny + j];
        }

        // Output results to file
        if (t % output_freq == 0)
        {
            std::ofstream file("output_" + std::to_string(t) + ".txt");
            for (int j = 0; j < Ny; j++)
            {
                for (int i = 0; i < Nx; i++)
                {
                    file << i * dx << " " << j * dy << " " << u[i * Ny + j] << " " << v
    [i * Ny + j] << "\n";
                }
                file << "\n";
            }
            file.close();
        }
    }
}

int main()
{
    // Simulation parameters
    const int Nx = 64;              // Number of grid points in the x-direction
    const int Ny = 64;              // Number of grid points in the y-direction
    const double Lx = 2.0 * M_PI;   // Length of the domain in the x-direction
    const double Ly =
```

As can be seen through this example, ChatGPT stops responding for producing relatively long codes. After each interruption, we ask ChatGPT to continue coding; however, this process is frustrating. Moreover, although it seems that ChatGPT tries to complete the rest of the code generated from the previous part, ChatGPT misses some intermediate codes in practice. For example, in the above example, ChatGPT stopped coding the section associated with "Set boundary conditions for u_star". After we asked it to continue coding, ChatGPT started coding the new section of "Solve tridiagonal system for u_star". At least for this case, we could not eventually

get a full C++ code from ChatGPT for solving the two-dimensional incompressible flow and the mission failed.

## 9.6 Default version (3.5) versus plus version (4.0) of ChatGPT

Currently, the default version (3.5) of ChatGPT is free. There is a possibility for users to upgrade ChatGPT to its "plus" version (4.0) with the cost of $20 per month subscription. However, we observe all the above-mentioned issues and failures even with the plus version of ChatGPT. It is worthwhile to note that there are significant differences between ChatGPT 3.5 and ChatGPT 4.0, based on the OpenAI company. Accordingly, it is claimed that ChatGPT 4.0 has a score of 5.0 out of 5.0 for "reasoning", while this score is equal to "3.0" for ChatGPT 3.5. Concerning "speed", the score of ChatGPT 4.0 is 2.0 out of 5.0, whereas the score of ChatGPT 3.0 is 5.0. Finally, the score of ChatGPT 4.0 and ChatGPT 3.5 for "conciseness" is 4.0 and 2.0 out of 5.0, respectively. Hence, users might select a suitable version according to their needs and tasks.

# 10 Summary

The most important messages of this technical report are summarized as follows. We demonstrate that using ChatGPT (provided by OpenAI), one can:

- Generate codes for implementing numerical algorithms in different programming languages such as C, C++, Python, MATLAB, Julia, etc; with specifying details such as boundary and initial conditions for partial differential equations
- Debug codes, improve code efficiency and complete incomplete codes of numerical methods
- Make C++ codes parallel using OpenMP
- Rewrite a given code in a different programming language

Additionally, the most important limitations and challenges of using ChatGPT for programming numerical algorithms discussed in this technical report are be listed as follows:

- Generating singular matrices (non-invertible)
- Producing arrays with incompatible sizes and shapes
- Irregular interruption for generating long codes, which are usually required for important and serious scientific simulations
- Including unknown libraries
- The lack of ability to recognize if a code is generated by humans or by itself (i.e., ChatGPT)

We plan to update this technical report on new findings. Additionally, we investigate the ChatGPT capacity for implementing other important numerical algorithms such as level set methods [33, 31, 39, 32], spectral methods [6], the smoothed particle hydrodynamics (SPH) method [46], point-cloud deep learning methodologies for computational mechanics [25, 22, 36, 35], the discontinuous Galerkin method [8, 10], etc.

# 11 Code availability

All the codes (including correct, incomplete, and buggy ones) are available on the following GitHub repository: https://github.com/Ali-Stanford/ChatGPT_Programming_Numerical_Methods

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