Problem 1 (10 points)
Obtain a general feeling of numerical physics. Please summarize the major models and algorithms in any book of ”numerical methods”.

答：
A general feeling of numerical physics:
用数值方法为无法解析求解的物理问题给出一个实用的结果。

Major models and algorithms:
插值，拟合，搜索，数值积分/微分，迭代求解本征值，龙格库塔求解 ode，蒙特卡罗，FFT 滤波/频谱分析，训练神经网络等等。

Problem 2 (10 points)
Summary the models in physics. Please summary as many models as possible in the books you have, which need to be calculated numerically. Models from literature are also welcome. The techniques in solving these problems are the focus of this course.

答：
牛顿力学下耦合多体系统的演化
非线性势场下系统的演化
天体运行轨道/航天器轨道的计算
计算流体力学
空气动力学
建筑的力学设计/有限元分析
软物质
大气/天线/微腔/FET 等等许多场合中的电磁场模拟
分子动力学模拟
密度泛函理论
药物设计
强关联体系
……

Problem 3 (10 points)
Analytical programming language. MATHEMATICA is very important in this course because a lot of calculations need to be done based this software. So install MATHEMATICA in your own computer; and summary the major commands in MATHEMATICA from the textbooks. Try some of them in your own computer.

答：
在附件中尝试了一些简单的指令。

Problem 4 (20 points)

Tricks in numerical calculations: I use the following simple, but important examples, to illustrate some importance tricks in numerical and analytical calculations, which will be frequently used in this course.

1. Please generate numbers xi and yi , where i = 1 − L (with L = 10000), then calculate

$$z = \prod x_i + \prod y_i$$

答：

$$z = z_1 + z_2 = 10^{\sum \log_{10}(x_i)} + 10^{\sum \log_{10}(y_i)}$$

令

$$z_1 = b_1 \times 10^{a_1}$$
$$z_2 = b_2 \times 10^{a_2}$$
$$z = b \times 10^{a}$$

令$a_1 \geq a_2$

$$b \times 10^{a} = (b_1 + b_2 \times 10^{a_2 - a_1}) \times 10^{a_1}$$

matlab code:

```
L=10000;


xi=5*rand(1,L)+1;
yi=6*rand(1,L)+2;


lgxi=sum(log10(xi));
lgyi=sum(log10(yi));


a1=floor(lgxi);
b1=10^(lgxi-a1);
a2=floor(lgyi);
b2=10^(lgyi-a2);


if a1<a2
    at=a1;bt=b1;
    a1=a2;b1=b2;
    a2=at;b2=bt;
end


a=a1;
b=b1+b2*10^(a2-a1);
```

```
if b>=10
    b=b/10;
    a=a+1;
end


fprintf('z = %f * 10 ^ %d\n',b,a);
```

输出：
z = 2.339708 * 10 ^ 6717

2. Please plot the following function

$$P(x) = \sum_{k=1}^{\infty} \frac{x^{\frac{k}{2}}}{(3k)!} \quad , x = 1, 2, 3, \ldots, 1000$$

答：
Stirling's approximation:

$$(3k)! \approx \sqrt{6\pi k}\left(\frac{3k}{e}\right)^{3k}$$

当$x \le 1000$

$$\frac{x^{\frac{k}{2}}}{(3k)!} \approx \frac{x^{\frac{k}{2}}}{\sqrt{6\pi k}\left(\frac{3k}{e}\right)^{3k}} = \frac{1}{\sqrt{6\pi k}\left(\frac{3k}{e \times x^{\frac{1}{6}}}\right)^{3k}} \le \frac{1}{\sqrt{6\pi k}\left(\frac{k}{2.87}\right)^{3k}}$$

对于$k \ge 10$

$$\sum_{k=10}^{\infty} \frac{x^{\frac{k}{2}}}{(3k)!} \le \sum_{k=10}^{\infty} \frac{1}{\sqrt{6\pi \times 10}\left(\frac{10}{2.87}\right)^{3k}} = 3.97 \times 10^{-18} \sum_{k=0}^{\infty} \frac{1}{42.14^{k}} = 4.07 \times 10^{-18}$$

所以计算 k<=9 时的求和就有足够高（~10^-18）的精度

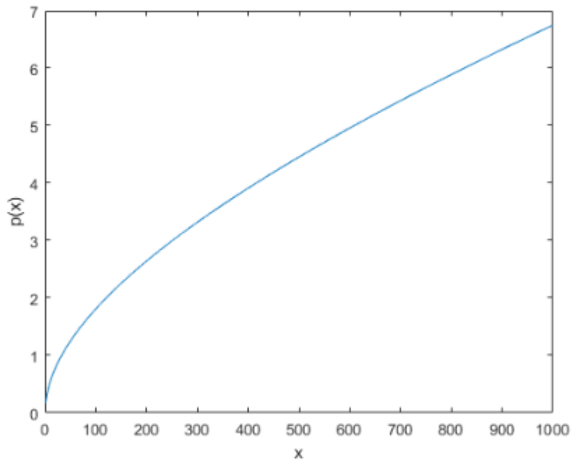
matlab code:

```
x=1:1000;
k=1:9;
[X,K]=meshgrid(x,k);


pxk=X.^(K/2)./factorial(3*K);
px=sum(pxk,1);
```

```
plot(x,px);
xlabel('x');ylabel('p(x)');
```

输出：



3. Determine the approximate polynomial of P(x), with error less than 10^−10 for x ∈ (0, 1000).

答：

由 2，k<=9 时的求和就有~10^-18 的精度

$$P(x)=\sum_{k=1}^{\infty}\frac{x^{\frac{k}{2}}}{(3k)!}\approx\sum_{k=1}^{9}p_k x^{\frac{k}{2}}$$

$$p_k=\frac{1}{(3k)!}$$

matlab code:

```
k=1:9;
pk=1./factorial(3*k);
fprintf('p_k, k = 1~9\n',b,a);
fprintf('%e\n',pk);
```

输出：

p_k, k = 1~9
1.666667e-01
1.388889e-03
2.755732e-06
2.087676e-09
7.647164e-13
1.561921e-16

1.957294e-20
1.611738e-24
9.183690e-29

4. About the Stirling's approximation for n!

$$n! = \sqrt{2\pi n}\left(\frac{n}{e}\right)^n \times F(n)$$

$$F(n) = 1 + \frac{1}{12n} + \frac{a_2}{n^2} + \frac{a_3}{n^3} + \frac{a_4}{n^4} + \cdots$$

Please determine the values of ai ∈ Z in the higher-order terms by numerical method.

答：

$$F(n) = \frac{n!}{\sqrt{2\pi n}\left(\frac{n}{e}\right)^n} = \frac{1}{\sqrt{2\pi n}}\exp\left(-n\ln\left(\frac{n}{e}\right) + \sum_{i=1}^{n}\ln(i)\right)$$

令

$$F(n) = a_0 + \frac{a_1}{n} + \frac{a_2}{n^2} + \frac{a_3}{n^3} + \frac{a_4}{n^4} + \cdots$$

$$F_1(n) = (F(n) - a_0) \times n = a_1 + \frac{a_2}{n} + \frac{a_3}{n^2} + \frac{a_4}{n^3} + \cdots$$

$$F_2(n) = (F_1(n) - a_1) \times n = a_2 + \frac{a_3}{n} + \frac{a_4}{n^2} + \frac{a_5}{n^3} + \cdots$$

$$F_{k+1}(n) = (F_k(n) - a_k) \times k = a_{k+1} + \frac{a_{k+2}}{n} + \frac{a_{k+3}}{n^2} + \frac{a_{k+4}}{n^3} + \cdots$$

通过$F_k(n)$的渐近线可以得到a_k

前 4 阶为

$$F(n) \approx 1 + \frac{1}{12n} + \frac{3.47 \times 10^{-3}}{n^2} + \frac{-2.7 \times 10^{-3}}{n^3} + \cdots$$

$$a_0 = 1, a_1 = \frac{1}{12}, a_2 \approx 3.47 \times 10^{-3}, a_3 \approx -2.7 \times 10^{-3}$$

matlab code:

```
N=1000;

x=1:N;
Fn=zeros(1,N);
an=zeros(1,order);


for ii=1:N
    lg=-ii*log(ii/exp(1))+sum(log(1:ii));
    Fn(ii)=1/sqrt(2*pi*ii)*exp(lg);
end
```

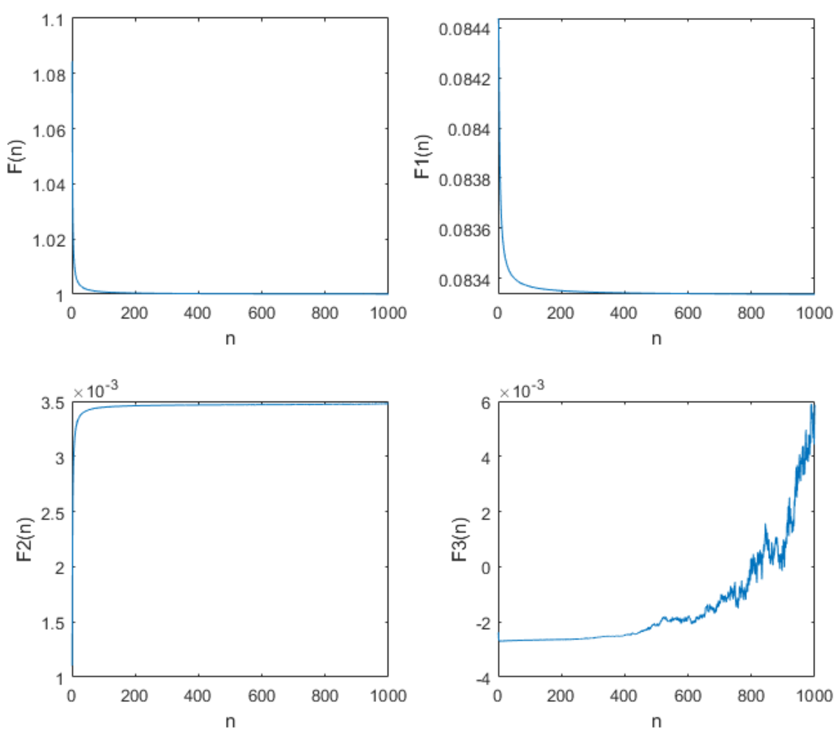
```
subplot(2,2,1);
plot(x,Fn);
xlabel('n');ylabel('F(n)');


F1n=(Fn-1).*x;
subplot(2,2,2);
plot(x,F1n);
xlabel('n');ylabel('F1(n)');


F2n=(F1n-1/12).*x;
subplot(2,2,3);
plot(x,F2n);
xlabel('n');ylabel('F2(n)');


F3n=(F2n-0.003472).*x;
subplot(2,2,4);
plot(x,F3n);
xlabel('n');ylabel('F3(n)');
```

输出：



要得到更高阶的系数应该要对调和级数求和的精度做优化。

5. Consider the Morse potential

$$V(r) = U\left(1 - \exp\left(-a(r - r_e)\right)\right)^2 - Fr, U, a, r_e > 0$$

Assume that F → 0, find analytically the minimal position of V (r), to the accuracy of F^3 , that is, V ′ (x) = 0, with

$$x = r_e + a_1 F + a_2 F^2 + a_3 F^3$$

Then determine ai analytically using perturbation theory; and verify them numerically.

答：

$$V(r) = U\left(1 - e^{-a(r-r_e)}\right)^2 - Fr$$

$$V'(r) = -F - 2\,a\,U\,\mathrm{e}^{-a\,(r-r_e)}\left(\mathrm{e}^{-a\,(r-r_e)} - 1\right)$$

对极小值点$V'(x) = 0$

$$\mathrm{e}^{-a\,(x-r_e)}\left(1 - \mathrm{e}^{-a\,(x-r_e)}\right) = \frac{F}{2\,a\,U}$$

$$1 - \mathrm{e}^{-a\,(x-r_e)} = \frac{1}{2} \pm \sqrt{\frac{1}{4} - \frac{F}{2\,a\,U}}$$

考虑$x - r_e \to 0$

$$1 - \mathrm{e}^{-a\,(x-r_e)} = \frac{1}{2} - \frac{1}{2}\sqrt{1 - \frac{2F}{a\,U}}$$

令$a\,(x - r_e) = \delta$, $\frac{2F}{a\,U} = \Delta$

$$1 - \mathrm{e}^{-\delta} = \frac{1}{2}\sqrt{1+\Delta} - \frac{1}{2}$$

$$\delta - \frac{\delta^2}{2} + \frac{\delta^3}{6} - \cdots = \frac{1}{4}\Delta + \frac{1}{16}\Delta^2 + \frac{1}{32}\Delta^3$$

其中

$$\delta = aa_1F + aa_2F^2 + aa_3F^3$$
$$\delta^2 = a^2a_1^2F^2 + 2a^2a_1a_2F^3 + o(F^4)$$
$$\delta^3 = a^3a_1^3F^3 + o(F^4)$$

$$aa_1F = \frac{1}{4}\Delta$$

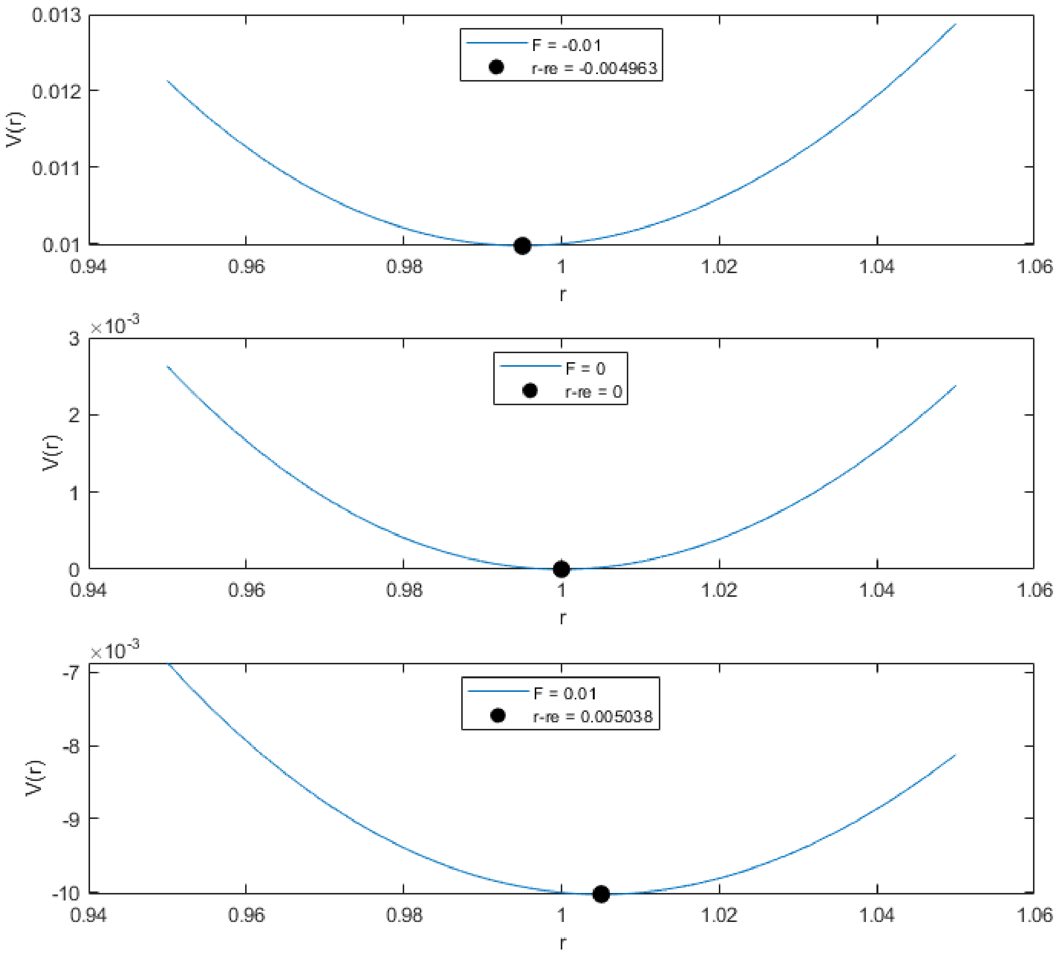
$$aa_2F^2 - \frac{1}{2}a^2a_1^2F^2 = \frac{1}{16}\Delta^2$$

$$aa_3F^3 - a^2a_1a_2F^3 + \frac{1}{6}a^3a_1^3F^3 = \frac{1}{32}\Delta^3$$

解得

$$a_1=\frac{1}{2}\frac{1}{a^2U},a_2=\frac{3}{8}\frac{1}{a^3U^2},a_3=\frac{5}{12}\frac{1}{a^4U^3}$$

取$U=1,a=1,r_e=1,\mathrm{F}=-0.01,0,0.01$，得到的势阱如下



直接搜索最小值， $\mathrm{F}=-0.01,0,0.01$时$x-r_e$分别为

$$-4.963\times10^{-3},0,5.038\times10^{-3}$$

而按三阶展开得到的$x-r_e$分别为

```
x=[-.01 0 .01];
(1/2*x+3/8*x.^2+5/12*x.^3)*1000
```

$$-4.963\times10^{-3},0,5.038\times10^{-3}$$

前四位完全一致。