

B. Herman and J. Roberts

Nuclear Reactor Core Methods

April 13, 2012

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Lists of abbreviations, symbols and the like are easily formatted with the help of the Springer-enhanced `description` environment.

PWR	Pressurized Water Reactor
BWR	Boiling Water Reactor
ANM	Analytic Nodal Method

Part I

Fundamentals

Lorem ipsum...

Chapter 1

Neutron Transport Equation

Abstract Each chapter should be preceded by an abstract (10–15 lines long) that summarizes the content. The abstract will appear *online* at www.SpringerLink.com and be available with unrestricted access. This allows unregistered users to read the abstract as a teaser for the complete chapter. As a general rule the abstracts will not appear in the printed version of your book unless it is the style of your particular book or that of the series to which your book belongs.

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1.1 Terminology

Definition of all terms (flux, current etc.) Just a copy paste of 106 notes I am sure

1.2 Derivation of Neutron Transport Equation

Jeremy I am sure you have this done from 106.

Chapter 2

Neutron Diffusion Equation

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2.1 Continuous Energy Diffusion Equation

This section will contain the derivation of the continuous form of the diffusion equation from the neutron transport equation.

Chapter 3

Multigroup Neutron Diffusion Equation

Abstract Each chapter should be preceded by an abstract (10–15 lines long) that summarizes the content. The abstract will appear *online* at www.SpringerLink.com and be available with unrestricted access. This allows unregistered users to read the abstract as a teaser for the complete chapter. As a general rule the abstracts will not appear in the printed version of your book unless it is the style of your particular book or that of the series to which your book belongs.

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3.1 Derivation of Multigroup Diffusion Equation

This section will contain the derivation of the multigroup diffusion equation from the continuous energy diffusion equation

Chapter 4

Finite Difference Methods

4.1 Taylor Series

The finite difference method relies heavily on the mathematical concept of Taylor Series. If we take a function, $f(x)$, the independent variable x can be discretized into many points as shown in Figure . If the value of the function is known at x_i , the value at x_{i+1} can be determined by a Taylor series expansion at x_i ,

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \dots + \frac{f^{(n)}(x_i)}{n!}h^n + \dots \quad (4.1)$$

In Eq. (4.1), $f^{(n)}$ represents the n -th derivative of the function and h is the spacing between points, $h = x_{i+1} - x_i$.

The expansion shown above is exact if the number of terms in the Taylor series expansion is taken to infinity. Of course, this is not practical for computational methods and therefore we truncate the series at a finite number of terms. The error present caused by the truncation is known as truncation error. Instead of representing the full Taylor expansion of a function, we will truncate the expression after a few number of terms and represent the truncation error with $\mathcal{O}(h^n)$. In this representation of the truncation error, n represents the order of convergence. Order of convergence means that as the grid is refined by a factor of two for example, the truncation error will reduce on the order of 2^n . This does not imply that one method is better than the other, just merely a concept of convergence rate due to truncation effects. Linear convergence is when $n = 1$, quadratic when $n = 2$ and cubic when $n = 3$. For example, if we expand a function to second order, we would rewrite Eq. (4.1) this as

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \mathcal{O}(h^3). \quad (4.2)$$

As we approximate differentials, we can keep track of this truncation error to determine order of convergence of our methods. This is one way to ensure that our discretization method and implementation of solution algorithms are correct.

4.2 Approximation of First Derivatives

There are many different approximations of differentials that can be constructed based on Taylor series. We will first consider the approximation of first order derivatives. The first approximation is a *first order forward difference* where we use information about a point just to the right, x_{i+1} , to infer the derivative at x_i . If we perform a Taylor expansion about point x_{i+1} to first order we get

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \mathcal{O}(h^2). \quad (4.3)$$

This equation can be solved for the derivative of the function at x_i

$$f'_{for}(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \mathcal{O}(h), \quad (4.4)$$

where $f'_{for}(x_i)$ represents the first order forward difference approximation to the derivative at x_i .

The opposite approximation is to consider a point to the left, x_{i-1} , to infer the derivative at x_i , known as the *first order backward difference*. Here, we take a Taylor expansion to the left,

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \mathcal{O}(h^2). \quad (4.5)$$

Solving for the derivative we can arrive at

$$f'_{bac}(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + \mathcal{O}(h). \quad (4.6)$$

Comparing Eqs. (4.4) and (4.6) we see that the formulation looks the same in that it is always the right point minus the left point in the numerator of the fraction. The only difference is the sign in the truncation error is reversed. Therefore, we can expect that one of these approximations will under-predict the true answer and the other one will over-predict. Again both of these methods are first order methods.

The last simple approximation of a first derivative is a *second-order central difference*. In this method we look at both left and right points. We can Taylor expand each of these to second order to get

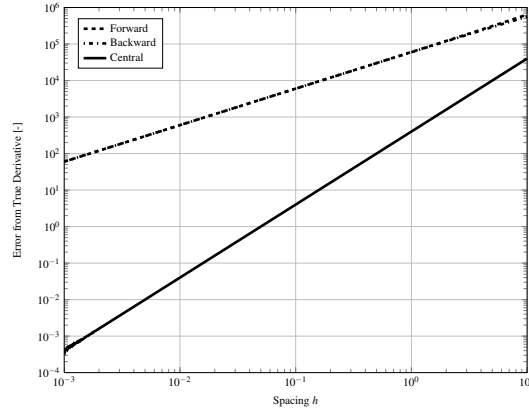
$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \mathcal{O}(h^3) \quad (4.7)$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \mathcal{O}(h^3). \quad (4.8)$$

Subtracting the x_{i-1} equation from the x_{i+1} , we are left with

$$f(x_{i+1}) - f(x_{i-1}) = 2f'(x_i)h + \mathcal{O}(h^3). \quad (4.9)$$

Fig. 4.1 Convergence rate of forward, backward and central difference approximations. The slope of the error as a function of mesh spacing is an estimate of the order of convergence of an approximation scheme.



Solving for the derivative at x_i we arrive at the second order central difference approximation

$$f'_{cen}(x_i) = \frac{f(x_{i+1}) - f(x_{i-1}))}{2h} - \mathcal{O}(h^2). \quad (4.10)$$

From the resulting expression, this approximation method does not depend on the value of the function at x_i and that the scheme is second order convergent.

Example - Order of Convergence First Derivative

As a simple example, we can approximate the derivative of the function, $f(x) = x^4$, at $x = 100$ with each of the above approximations. We can choose an array of spacing values between x_i and x_{i+1} and x_{i-1} and x_i . For each spacing value we compute the estimate of the derivative using the three approximations above. To characterize the error of each we find the absolute difference between the approximation and the true value of the derivative at $x = 100$. To infer the order of convergence, we can graph the errors as a function of spacing on a log-log scale. These convergence plots are shown in Fig. 4.1.

There are two distinct convergence trends present in Fig. 4.1. The curve with a slope of 1 on the log-log scale represents forward and backward finite difference approximations. This shows that these methods have linear convergence consistent with the truncation error. For the central difference approximation we predicted that it would have quadratic convergence. We can see from the plot that the magnitude of the slope is 2 on the log-log scale. MATLAB code to solve generate this plot is included below.

```
% Simple Approximation of First Order Derivative

% Function
f = @(x) x.^4;
```

```

% Analytical Derivative of Function
df_exact = @(x) 4*x.^3;

% Create a log space of h (width between x values)
h = logspace(-3,1,1000);

% Perform approximation with forward finite difference
df_for = (f(100+h) - f(100))./h;

% Perform approximation with backward finite difference
df_bac = (f(100) - f(100-h))./h;

% Perform approximation with central finite difference
df_cen = (f(100+h) - f(100-h))./(2*h);

% Compute Error
err_for = abs(df_for - df_exact(100));
err_bac = abs(df_bac - df_exact(100));
err_cen = abs(df_cen - df_exact(100));

% Plot Results
loglog(h,err_for,'k--','LineWidth',2);
hold on
loglog(h,err_bac,'k-','LineWidth',2);
loglog(h,err_cen,'k-','LineWidth',2);
grid
grid minor
xlabel('x spacing [-]','LineWidth',2);
ylabel('Error from true derivative [-]');
legend('Forward','Backward','Central','Location','NorthWest');

```

4.3 Approximation of Second Derivatives

In nuclear reactor physics applications, we also need approximations for second derivatives. The only difference in these approximations is that more points to the left or right of x_i need to be included. For the *first order forward difference* approximation, we write two equations to second order. One equation representing a Taylor expansion to x_{i+1} and the other to x_{i+2} ,

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \mathcal{O}(h^3) \quad (4.11)$$

$$f(x_{i+2}) = f(x_i) + f'(x_i)(2h) + \frac{f''(x_i)}{2!}(2h)^2 + \mathcal{O}(h^3). \quad (4.12)$$

Since we are approximating the second derivative, the first derivative needs to be canceled out. To cancel this term out, we multiply Eq. (4.11) by a 2 and subtract it from Eq. (4.12). The resulting expression is

$$f(x_{i+2}) - 2f(x_{i+1}) = -f(x_i) + f''(x_i)h^2 + \mathcal{O}(h^3). \quad (4.13)$$

The approximation of the second derivative for a first-order forward difference is therefore

$$f''_{for}(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} - \mathcal{O}(h). \quad (4.14)$$

For the *first-order backward finite difference* approximation of the second derivative we Taylor expand the function at x_{i-1} and x_{i-2}

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \mathcal{O}(h^3) \quad (4.15)$$

$$f(x_{i-2}) = f(x_i) - f'(x_i)(2h) + \frac{f''(x_i)}{2!}(2h)^2 - \mathcal{O}(h^3). \quad (4.16)$$

Similar to the forward finite difference case, we must eliminate the first derivative term by multiplying Eq. (4.15) by 2 and subtract from Eq. (4.16). This results in the following expression:

$$f(x_{i-2}) - 2f(x_{i-1}) = -f(x_i) + f''(x_i)h^2 - \mathcal{O}(h^3). \quad (4.17)$$

The approximation of the second derivative for a first-order backward difference is therefore

$$f''_{bac}(x_i) = \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2} + \mathcal{O}(h). \quad (4.18)$$

Lastly, the *second-order central difference* approximation to the second derivative can be derived by performing a Taylor expansion at x_{i-1} and x_{i+1} to fourth-order,

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \mathcal{O}(h^4) \quad (4.19)$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \mathcal{O}(h^4). \quad (4.20)$$

To eliminate the first derivative term, these two equations can be directly added together resulting in

$$f(x_{i+1}) + f(x_{i-1}) = 2f(x_i) + f''(x_i)h^2 + \mathcal{O}(h^4). \quad (4.21)$$

The approximation of the second derivative for a second-order central difference is

$$f''_{cen}(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1}))}{h^2} - \mathcal{O}(h^2). \quad (4.22)$$

The second-order central difference will be the main approximation we use for second order derivatives. This is mainly due to the fact that has quadratic convergence. The other reason is that for a given computational node in a reactor, we think of

leakage occurring to the left and to the right. This leakage term is represented with mathematically by a second derivative and by using the central difference approximation, we can couple to both the right and left nodes.

Example - Order of Convergence First Derivative

4.4 Higher Order Finite Difference

4.5 Nonuniform Spacing

4.6 Finite Difference Multigroup Diffusion Equation

Chapter 5

Finite Volume Methods

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Chapter 6

Finite Element Methods

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Chapter 7

Stationary Iterative Methods

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This chapter will contain the idea of iterative methods, and talk about Jacobi and Gauss - Siedel, example should be provided either for fission source iterations or energy group sweep. Also should include SOR method.

Chapter 8

Nonstationary Iterative Methods - Krylov Subspace Methods

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REF: <http://www.netlib.org/utk/papers/templates/node9.html>

Intro to Krylov Methods Arnoldi Iterations - Gram-Schmidt etc?

Chapter 9

Conjugate Gradient

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Specific example - Conjugate Gradient

Chapter 10

GMRES

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REF: <http://www.netlib.org/utk/papers/templates/node9.html>

Specifically derive out GMRES with givens rotations. Preconditioning JFNK?

Chapter 11

Power Iteration

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Derive out the power iteration method and give example.

Chapter 12

Nonlinear Iteration

Abstract Each chapter should be preceded by an abstract (10–15 lines long) that summarizes the content. The abstract will appear *online* at www.SpringerLink.com and be available with unrestricted access. This allows unregistered users to read the abstract as a teaser for the complete chapter. As a general rule the abstracts will not appear in the printed version of your book unless it is the style of your particular book or that of the series to which your book belongs.

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Newton Iteration - with GMRES JFNK

Chapter 13

Chebyshev Acceleration Method

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Chebyshev Acceleration of Power iteration

Chapter 14

Time Stepping Methods

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Forward Euler (Explicit) Backward Euler (Implicit) Runge-Kutta (4th order mostly used in spatial kinetics) Adams-Moulton Adams-Bashforth

Part II

Reactor Statics

Lorem ipsum...

Chapter 15

Classical Nodal Methods - Flare Model

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Summer course on nodal methods (Herman office)

Chapter 16

Analytic Nodal Method

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Derivation of Analytic Nodal Method with example code Smith Master Thesis

Chapter 17

Nodal Expansion Method

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- Bandini Thesis

Part III
Reactor Dynamics

Lorem ipsum...

Appendix A

Chapter Heading

All's well that ends well

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A.1 Section Heading

Instead of simply listing headings of different levels we recommend to let every heading be followed by at least a short passage of text. Furtheron please use the L^AT_EX automatism for all your cross-references and citations.

A.1.1 Subsection Heading

Instead of simply listing headings of different levels we recommend to let every heading be followed by at least a short passage of text. Furtheron please use the L^AT_EX automatism for all your cross-references and citations as has already been described in Sect. A.1.

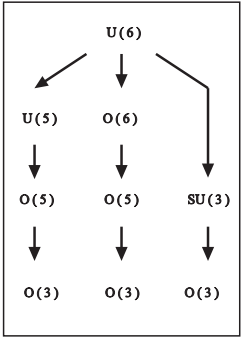
For multiline equations we recommend to use the `eqnarray` environment.

$$\begin{array}{l} \mathbf{a} \times \mathbf{b} = \mathbf{c} \\ \mathbf{a} \times \mathbf{b} = \mathbf{c} \end{array} \quad (\text{A.1})$$

A.1.1.1 Subsubsection Heading

Instead of simply listing headings of different levels we recommend to let every heading be followed by at least a short passage of text. Furtheron please use the

Fig. A.1 Please write your figure caption here



L^AT_EX automatism for all your cross-references and citations as has already been described in Sect. A.1.1.

Please note that the first line of text that follows a heading is not indented, whereas the first lines of all subsequent paragraphs are.

Table A.1 Please write your table caption here

Classes	Subclass	Length	Action Mechanism
Translation	mRNA ^a	22 (19–25)	Translation repression, mRNA cleavage
Translation	mRNA cleavage	21	mRNA cleavage
Translation	mRNA	21–22	mRNA cleavage
Translation	mRNA	24–26	Histone and DNA Modification

^a Table foot note (with superscript)

Glossary

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