第2章 非线性方程的数值解法

(2) Newton迭代法

简单迭代法回顾

迭代公式： $x_{k+1} = \varphi(x_k)$

收敛性： $|\varphi'(x)| \le L < 1$

收敛速度： $\lim\limits_{k\to\infty} \dfrac{|e_{k+1}|}{|e_k|^p} = C \neq 0$ $\qquad e_k = x^* - x_k$

判断方法： $\varphi'(x^*) = \varphi''(x^*) = \ldots = \varphi^{(p-1)}(x^*) = 0$

$\varphi^{(p)}(x^*) \neq 0$

迭代加速方法:

改造迭代函数 $\phi(x)=\varphi(x)+\lambda[\varphi(x)-x]$ $\phi'(x^*)\approx 0$

$$\lambda=\frac{\varphi'(x^*)}{1-\varphi'(x^*)}\approx\frac{\varphi'(x_k)}{1-\varphi'(x_k)}$$

迭代公式:

$$\begin{aligned}x_{k+1}&=\phi(x_k)\\&=\varphi(x_k)+\lambda[\varphi(x_k)-x_k]\\&=(1+\lambda)\varphi(x_k)-\lambda\,x_k\end{aligned}$$

实质-加权平均: $\bar{x}_{k+1}=\varphi(x_k)$ ——— 原迭代公式

$$(1+\lambda)\bar{x}_{k+1}-\lambda x_k \longrightarrow x_k$$

Newton迭代法

简单迭代法是原来函数的等价变形:

$$f(x)=0 \Leftrightarrow x=\varphi(x)$$

$\varphi(x)$ 与 f 的导数无关

Newton迭代法中，迭代函数与 f 的导数无关，利用更多的函数信息，收敛更快

Joseph Raphson was an English mathematician known best for the Newton–Raphson method. Little is known about his life, and even his exact years of birth and death are unknown, although the mathematical historian Florian Cajori provided the approximate dates 1648–1715. Raphson attended Jesus College at Cambridge, graduating with an M.A. in 1692.[1] He was made a Fellow of the Royal Society on 30 November 1689, after being proposed for membership by Edmund Halley.

Raphson's most notable work is *Analysis Aequationum Universalis*, which was published in 1690. It contains a method, now known as the Newton–Raphson method, for approximating the roots of an equation. Isaac Newton had developed a very similar formula in his *Method of Fluxions*, written in 1671, but this work would not be published until 1736, nearly 50 years after Raphson's *Analysis*. However, Raphson's version of the method is simpler than Newton's, and is therefore generally considered superior. For this reason, it is Raphson's version of the method, rather than Newton's, that is to be found in textbooks today.

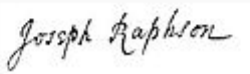
Raphson was a staunch supporter of Newton's claim, and not that of Gottfried Leibniz, to be the sole inventor of calculus. In addition, Raphson translated Newton's*Arithmetica Universalis* into English.

Raphson coined the word *pantheism*, in his work *De Spatio Reali*, published in 1697,[2] where it may have been found by John Toland, who called Raphson's work "ingenious".[3] In *De Spatio Reali*, Raphson begins by making a distinction between atheistic *panhylists* (from the Greek *pan* 'all' and *hyle* 'wood, matter'), who believe everything derives from matter, and pantheists who believe in "a certain universal substance, material as well as intelligent, that fashions all things that exist out of its own essence".[4] Raphson further believed the universe to be immeasurable in respect to a human's capacity of understanding, and that humans will never be able to comprehend it.[5]

Joseph Raphson

Born	c. 1648 Middlesex, England
Died	c. 1715 England
Residence	England
Nationality	English
Fields	Mathematician
Alma mater	University of Cambridge
Known for	Newton–Raphson method

Signature



基本思想： 化繁为简，“简单”的重复

最简单的函数求根 $f(x)=ax+b$ 线性函数

如何利用线性函数逼近非线性函数

Taylor展开

$$f(x)=f(x_k)+f'(x_k)(x-x_k)+\frac{1}{2}f''(x_k)(x-x_k)^2+\ldots$$

$$f(x)\approx f(x_k)+f'(x_k)(x-x_k)$$

求根： $f(x_k)+f'(x_k)(x-x_k)\approx 0$

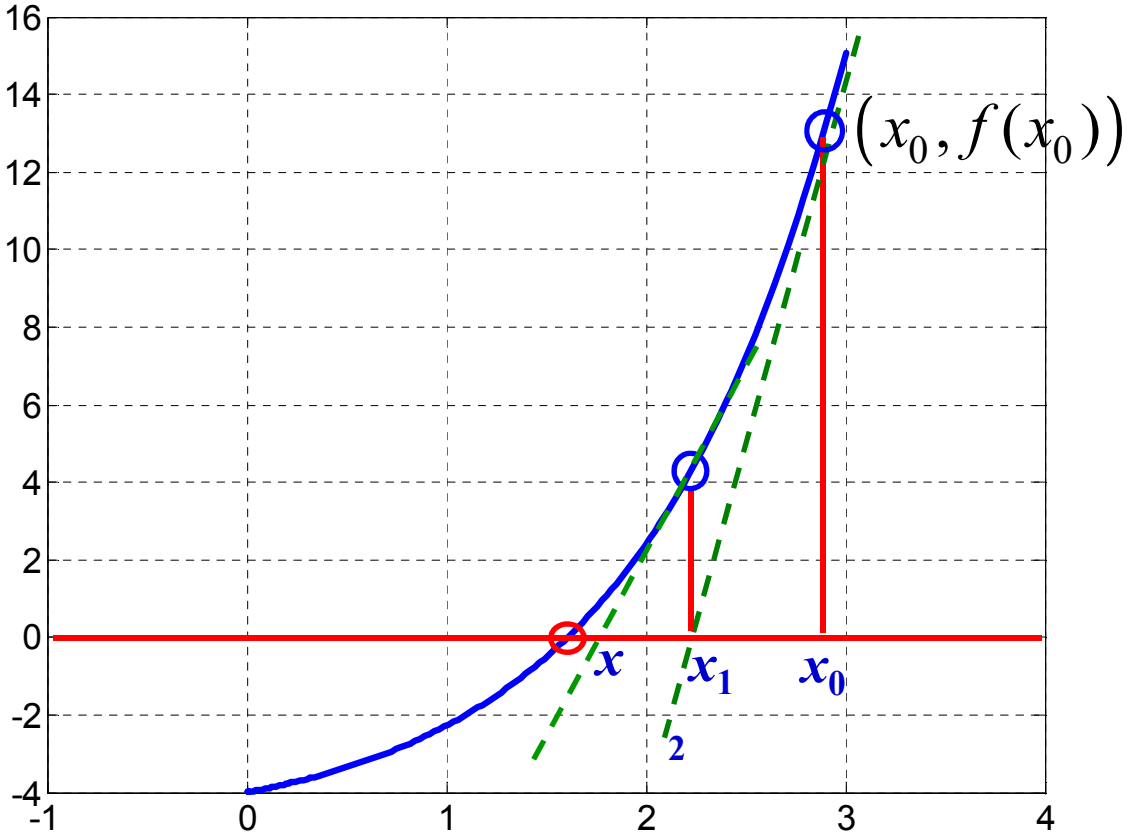
$$\bar{x}_{k+1} = \bar{x}^* \approx x_k - \frac{f(x_k)}{f'(x_k)}$$

线性方程的准确解

原函数准确解的近似

$$\rightarrow \quad x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

几何直观



收敛的充分条件：设 $f \in C^2[a,b]$，若

(1) $f(a)f(b) < 0$;

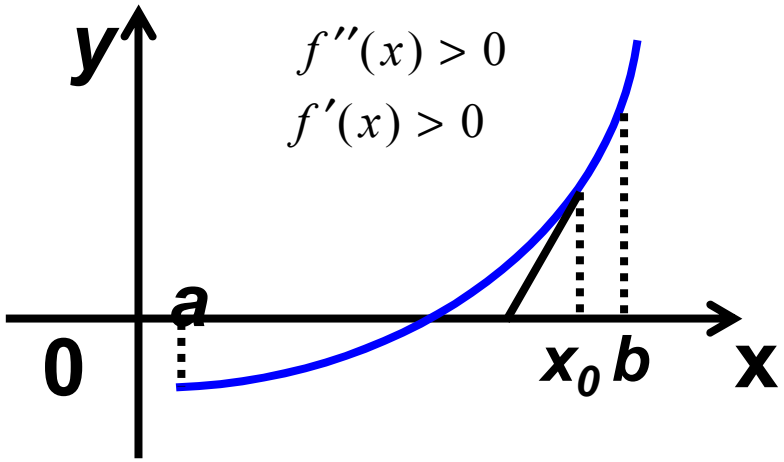
(2) 在整个$[a,b]$上 f''不变号且 $f'(x) \neq 0$;

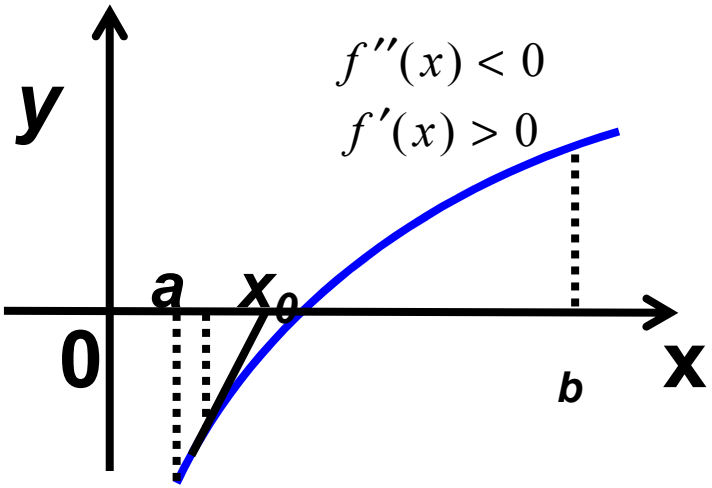
(3) 选取 $x_0 \in [a,b]$ 使得 $f(x_0)f''(x_0) > 0$;

$\{x_k\}$ 收敛到$f(x)$ 在 $[a,b]$ 的唯一根。

根唯一

产生的序列单调有界，保证收敛。


y
$f''(x) > 0$
$f'(x) > 0$
a
0
x_0 b
x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x_0
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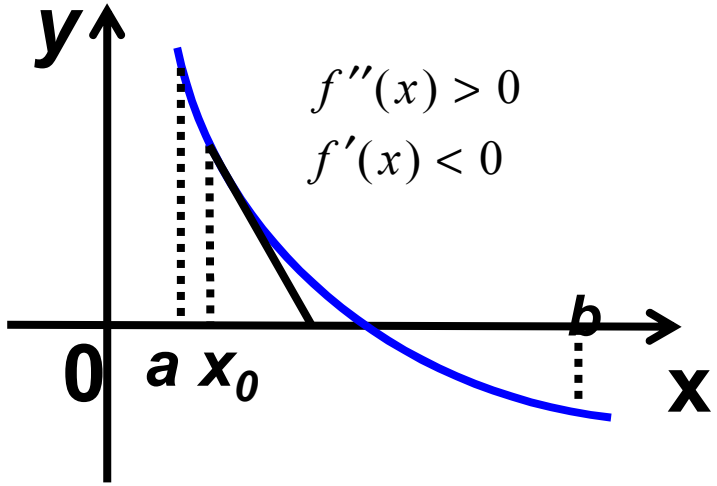
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$f''(x) > 0$
$f'(x) < 0$
b
0
a x_0
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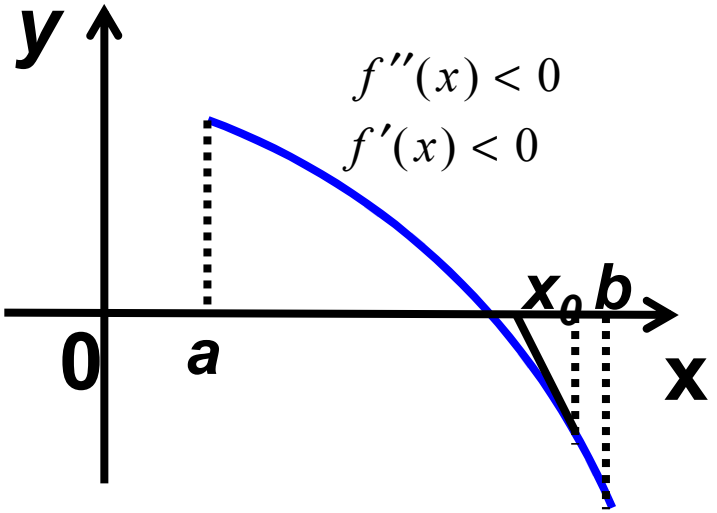

y
$f''(x) < 0$
$f'(x) < 0$
x_0 b
0
a
x

例　用迭代法求 $x^3-x^2-1=0$ 在隔根区间 $[1.4,1.5]$ 内的根，要求准确到小数点后第4位。

（1）牛顿迭代公式为

$$x_{n+1}=x_n-\frac{f(x_n)}{f'(x_n)}=x_n-\frac{x_n^3-x_n^2-1}{3x_n^2-2x_n}=\frac{2x_n^3-x_n^2+1}{3x_n^2-2x_n}$$

（2）$f(1.4)\approx -0.2$　　$f(1.5)\approx 0.2$

当 $x\in[1.4,1.5]$ 时有，

$$f'(x)=3x^2-2x>0 \qquad f''(x)=6x>0$$

因 $f(1.5)f''(1.5)>0$，故取 $x_0=1.5$，牛顿迭代法收敛。

$f(x)=x^3-x-1$

$f'(x)=3x^2-1=$

$f''(x)=6x$

$f(1)<0 \quad f(2)>0$

$f''(x)>0 \quad f(2)\checkmark$

$$x_{k+1}=x_k-\frac{x_k^3-x_k-1}{3x_k^2-1}$$

```
function y=newton(fname,dfname,x0,e,N)
y=x0;
x0=y+2*e;
k=0;
while abs(x0-y)>e&k<N
    k=k+1;
    x0=y;
    y=x0-fname(x0)/dfname(x0);
    disp(k,y)
end
if k==N
    disp('warning')
end
```

```
f=inline('x^3-x^2-1');
df=inline('3*x^2-2*x');
y=newton(f,df,1.5,0.5*10^(-4),500)
```

$x_1=1.34783$

k: 1 2 3

x: 1.4667

1.4656

1.4656

$x_2=1.32520$

$x_3=1.32472$

求$\sqrt{a}$牛顿迭代，

$f(x)=x^2-a$

$$x_{k+1}=x_k-\frac{x_k^2-a}{2x_k}$$

$$=\frac{x_k}{2}+\frac{a}{2x_k}$$

$x^2-a=0$

$a-$

? 利用抛物线近似

Newton方法事实上是一种特殊的不动点迭代

$$\varphi(x) = x - \frac{f(x)}{f'(x)}$$

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

$$|\varphi'(x^*)| = \left|\frac{f''(x^*)f(x^*)}{f'^2(x^*)}\right| = 0 < 1 \quad \Rightarrow \quad \text{收敛}$$

$$|\varphi''(x^*)| \neq 0$$

平方收敛

$$\varphi'(x) = 1 - \frac{f'^2(x) - f(x)f''(x)}{[f'(x)]^2} = \frac{f(x)f''(x)}{f'^2(x)}$$

$$f(x)=f(x_k)+f'(x_k)(x-x_k)+\frac{1}{2}f''(x_k)(x-x_k)^2=0.$$

$$\frac{1}{2}f''(\quad)x^2+[f'(x_k)-f''(x_k)x_k]x+[x_k^2-f'(x_k)x_k+f(x_k)]=0,$$

$$\Delta=[\quad]^2-2f''(\quad)x^2[x_k^2-f'(x_k)x_k+f(x_k)]=0.$$

牛顿迭代法的优缺点

1、优点：牛顿迭代法具有平方收敛的速度，所以在迭代过程中只要迭代几次就会得到很精确的解。这是牛顿迭代法比简单迭代法优越的地方。

2、缺点：选定的初值要接近方程的解，否则有可能得不到收敛的结果。再者，牛顿迭代法计算量比较大。因每次迭代除计算函数值外还要计算导数值

三种简化牛顿迭代法.

牛顿法主要有两个缺点：局部收敛，计算量大。

(1)简易Newton法

$$x_{k+1} = x_k - \frac{f(x_k)}{M} \qquad (k = 0,1,2,\cdots)$$

用M代替$f'(x_k)$

(2)割线法

$$x_{k+1} = x_k - \frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})} f(x_k) \qquad (k = 0,1,2,\cdots)$$

用割线斜率代替切线斜率.

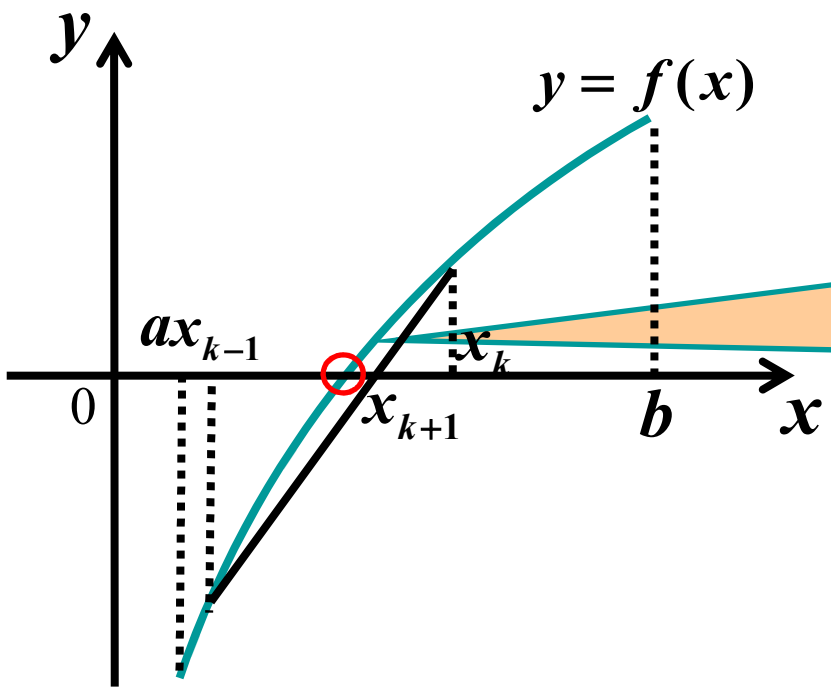
(3)牛顿下山法

$$x_{k+1} = x_k - \omega \frac{f(x_k)}{f'(x_k)} \qquad (k = 0,1,2,\cdots)$$

可引入一个下山因子$\omega(0 < \omega \leq 1)$,
使每一步有$|f(x_{k+1})| < |f(x_k)|$

最终达到$|f(x^*)| \approx 0$

割线法的几何意义



用割线代替曲线，用线性函数的零点作为*f(x)*的零点的近似值。

割线法

$$x_{k+1} = x_k - \frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})} f(x_k) \qquad (k = 0,1,2,\cdots)$$

收敛阶为 p=1.68

迭代方法总结

二分法	简单迭代法	Newton迭代法
使用：函数的符号	使用：迭代函数值	使用：迭代函数值 导数值
要求：函数连续	要求：迭代函数 的1阶导数	要求：迭代函数 的1阶和2阶导数
收敛：慢	收敛：依赖迭代函数	收敛：快(2阶)

Luc Mieussens Professor, Université de Bordeaux

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Luc Mieussens
Professor, Université de Bordeaux

DISCRETE VELOCITY MODEL AND IMPLICIT SCHEME FOR THE BGK EQUATION OF RAREFIED GAS DYNAMICS

The second aim of this paper is to provide a fast and robust algorithm for steady-state computations. Many numerical schemes have been proposed for unsteady BGK equation (see the references below), but the simulation of stationary flows involves additional difficulties. For these flows, one may either solve the steady BGK equation with an iterative scheme (due to the nonlinearity of the source term), or solve the unsteady equation and then let time evolve to infinity.

In the first method, the nonlinearity may be treated by a Newton algorithm, but it is well known in CFD that such a method is not very robust and may not converge. It may also be treated by a fixed point technique like Aoki, Kanba, Takata in [3] with the scheme $v \cdot \nabla_x f^{n+1} = \frac{1}{\tau^n}(M[f^n] - f^{n+1})$, but this leads to the uncoupling of the gain and loss terms, and may converge very slowly. This can be viewed as a semi-implicit method for the non-stationary equation where only the loss term $-f$ is implicit (because it gives negative distributions). In this paper, we demonstrate that this method is slow.

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methods are probabilistic, such as the Direct Simulation Monte Carlo (DSMC) method. The main drawback of these methods is the frequent occurrence of noisy

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An implicit kinetic scheme for multiscale heat transfe accounting for phonon dispersion and polarization

Chuang Zhang, Zhaoli Guo, Songze Chen*

State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology, Wuhan 430074, China

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Implicit kinetic scheme

ABSTRACT

An efficient implicit kinetic scheme is developed equation (BTE) based on the non-gray model with tion. Due to the wide range of the dispersed phor non-gray model is essentially multiscale, and has and branches. The proposed kinetic scheme is co iteration. The microscopic iteration is capable of a path of each phonon frequency and branch by solv is gathered together by the microscopic iteration t dicted by a macroscopic heat transfer equation acc phonon BTE is also updated. The combination of makes the present method very efficient in a wide the cross-plane, in-plane and nano-porous heat tr can handle the phonon dispersion and polarization nomena efficiently. Furthermore, the proposed me cit DOM while keeps the same amount of the mem transfer problems.

3.2. Macroscopic iteration

The corresponding macroscopic governing equation of Eq. (5) is

$$\nabla \cdot \boldsymbol{q} = 0, \tag{26}$$

where the heat flux $\boldsymbol{q} = \boldsymbol{q}(T)$ can be regarded as a functional of the temperature field $T(\boldsymbol{x})$ on a macroscopic view. Although no universal formula for the heat flux can be established at the micro/nano scale, $\boldsymbol{q}$ can be explicitly calculated by the moments of the distribution function in the framework of the phonon BTE. In the last subsection, the numerical heat flux is obtained by Eq. (24) in the microscopic iteration. Then a macroscopic residual is defined as

$$\mathrm{RES}^n = \mathrm{RES}(T^n) = -\nabla \cdot \boldsymbol{q}^{n+1}. \tag{27}$$

An approximate linear operator $(\tilde{Q})$ [37,46–48,34,36] is invoked and acts on the increment of the temperature δT,

$$\tilde{Q}(\delta T^n) = \mathrm{RES}^n, \tag{28}$$

so that $||\mathrm{RES}(T^n + \delta T^n)|| < ||\mathrm{RES}(T^n)||$, where $\delta T^n = T^{n+1} - T^{**}$, T^{**} is obtained by Eq. (23). As the residual goes to zero, Eq. (26) can be satisfied.

The formula of the approximate linear operator is

$$\tilde{Q}(\delta T) = \nabla \cdot (-\beta k_{\mathrm{bulk}} \nabla(\delta T)), \tag{29}$$

where β is a non-dimensional coefficient which can be adjusted to ensure the convergence of the iteration, and

$$k_{\mathrm{bulk}} = \frac{1}{3} \sum_p \int_{\omega_{\min,p}}^{\omega_{\max,p}} C|\boldsymbol{v}|^2 \tau d\omega \tag{30}$$

is the bulk thermal conductivity obtained in the diffusive limit. Based on the theorem of the inexact Newton method [46–48], the iteration may converge within a certain range of β. As long as the iteration converges, the approximate linear operator will not influence the final convergent solution. Without special statements, β is set to be a constant in the whole iterative process for simplicity.

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Unified implicit kinetic scheme for steady multiscale heat transfer based on the phonon Boltzmann transport equation

Chuang Zhang, Zhaoli Guo,* and Songze Chen†
State Key Laboratory of Coal Combustion, School of Energy and Power Engineering, Huazhong University of Science and Technology, Wuhan 430074, China
(Received 25 July 2017; published 21 December 2017)

An implicit kinetic scheme is proposed to solve the stationary phonon Boltzmann transport equation (BTE) for multiscale heat transfer problem. Compared to the conventional discrete ordinate method, the present method employs a macroscopic equation to accelerate the convergence in the diffusive regime. The macroscopic equation can be taken as a moment equation for phonon BTE. The heat flux in the macroscopic equation is evaluated from the nonequilibrium distribution function in the BTE, while the equilibrium state in BTE is determined by the macroscopic equation. These two processes exchange information from different scales, such that the method is applicable to the problems with a wide range of Knudsen numbers. Implicit discretization is implemented to solve both the macroscopic equation and the BTE. In addition, a memory reduction technique, which is originally developed for the stationary kinetic equation, is also extended to phonon BTE. Numerical comparisons show that the present scheme can predict reasonable results both in ballistic and diffusive regimes with high efficiency, while the memory requirement is on the same order as solving the Fourier law of heat conduction. The excellent agreement with benchmark and the rapid converging history prove that the proposed macro-micro coupling is a feasible solution to multiscale heat transfer problems.

DOI: 10.1103/PhysRevE.96.063311

I. INTRODUCTION

In recent years, much attention has been paid to the study of the thermal performance of micro- or nanoscale electronic devices [1,2]. It is well recognized that the traditional Fourier law cannot predict the heat transfer behaviors correctly when the characteristic length of the objects is comparable or smaller than the mean free path of heat carriers and/or the time scale

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A. Macroscopic implicit scheme

Considering a system without heat source, the first law of the thermodynamics at steady state can be written as

$$\nabla \cdot \boldsymbol{q} = 0, \tag{7}$$

where $\boldsymbol{q}$ depends on the distribution of T, namely, $\boldsymbol{q} = \boldsymbol{q}[T(\boldsymbol{x})]$. This equation is universally valid for all Knudsen numbers at steady state. Since the specific expression of $\boldsymbol{q}[T(\boldsymbol{x})]$ is unknown at the microscale, Eq. (7) cannot be solved directly. Therefore, we invoke the inexact Newton method [43–45] (see Appendix) to solve Eq. (7) iteratively. Define a residual as follows:

$$\mathrm{RES} = Q(T) = -\nabla \cdot \boldsymbol{q}, \tag{8}$$

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