A Coupled-Ordinates Method for the Boltzmann Transport Equation

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Introduction

The Boltzmann transport equation (BTE) is a general framework to characterize the transport of quantum particles through a semi-classical framework. With these particles (electrons, phonons, neutrons, etc.), the distribution function of particles in physical, temporal and phase space is found. For gas molecules, for example, the distribution function *f* (**r**,**v**,*t*) is a function of physical space and time, and in addition, velocity space. For phonons, the phase space is wave vector space. In a typical sequential solution procedure, at each time step, each point in phase space is visited in turn, solving all physical space. This leads to slow convergence due to strong inter-equation coupling caused by inter-particle scattering. The Coupled-Ordinates Method (COMET), addresses this issue by visiting each spatial point in turn, solving all points in phase space in point-coupled fashion. To promote the reduction of low wave-number errors, this point-coupled procedure is used as a relaxation sweep in a FAS multigrid procedure.

BTE

$$\frac{\partial f}{\partial t} + \vec{v}_g \cdot \nabla_{\vec{r}} f + \vec{F} \cdot \nabla_{\vec{k}} f = \left(\frac{\partial f}{\partial t}\right)_{scatt} \approx \frac{f^0 - f}{\tau}$$

f, f^0 – Non-equilibrium, equilibrium probability distribution function

$\vec{v}_g$ - Particle velocity

$\vec{F}$ - Force field vector

τ - Relaxation time

$\nabla_{\vec{r}}, \nabla_{\vec{k}}$ - Spatial and k-space gradient

Discretization

The BTE is discretized using a finite volume method in the spatial domain. For particles with trivial dispersion or an unbounded velocity space, it is best to use spherical coordinates in phase space. A finite volume discretization may be used to discretize direction, while any quadrature rule may be used to discretize magnitude. For particles, such as phonons with complicated dispersion and a finite k-space, a finite volume discretization can be used to discretize phase space.

Radiation Results*

This table shows the speedup obtained when solving for radiative intensity in a quadrilateral cavity with a Planck number = 1.4e-5 for different optical thicknesses

κL	Sequential CPU, s	Sequential Iterations	COMET CPU, s	COMET Iterations
650 Cells				
0.1*L*	11.25	12	12.4	5
1.0*L*	18.66	25	12.82	5
10.0*L*	144.06	239	16.45	5
2,600 Cells				
0.1*L*	98.53	12	81.85	5
1.0*L*	112.46	25	73.23	5
10.0*L*	690.99	252	72.65	5
10,400 Cells				
0.1*L*	488.57	12	376.99	5
1.0*L*	714.97	24	344.63	5
10.0*L*	3209.37	266	278.73	5

Optical thickness (inverse Knudsen number)

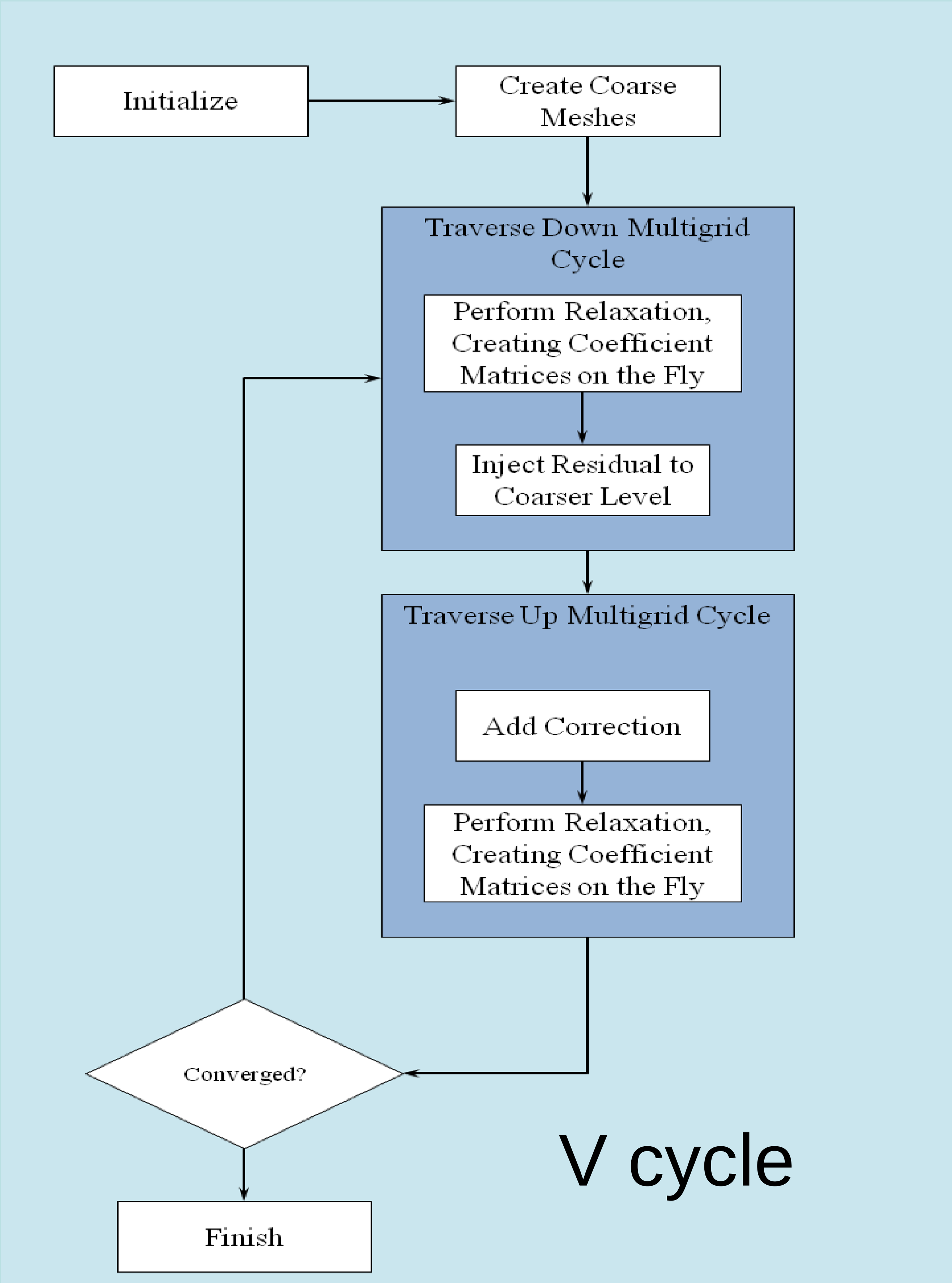
Uncertain Inputs

General Inputs
- -Boundary condition values
- -Domain geometry

BTE Inputs (when applicable)
- -Relaxation times
- -Force field vector
- -Dispersion relation

COMET

At each spatial point, all points in phase space are solved directly. A full approximation storage (FAS) multigrid scheme is used, with a block Gauss-Seidel scheme as the relaxation sweep. Because coefficient storage quickly becomes large, all coefficients are created on the fly at the different multigrid levels



V cycle

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*S. R. Mathur, J. Y. Murthy, Journal of Thermophysics and Heat Transfer, 1999, Vol. 12, No. 4, pp 467-473.