Performance Narrative for the NRC MSIP Grant for NY- Nuclear Research Opportunities Program (NY-NROP)

(October 1, 2011 - March 31, 2012) - prepared by M. Kawaji

This is the third progress report for the New York Nuclear Research Opportunities Program (NY-NROP) at The City College of New York funded by a grant from NRC's MSIP program covering the period from October 1, 2011 through March 31, 2012.

I. Specific Aims and Objectives

This program's objective is to enable a total of 5 Master of Engineering (M.Eng.) students and 1 Ph.D. student to conduct cutting edge research in the Nuclear Thermalhydraulics and Safety Research Laboratory at the Energy Institute located in the Grove School of Engineering at City College of New York in Manhattan, New York. This program aims at providing minority students with the research experience, advanced knowledge and skills needed to pursue successful careers in the nuclear industry, National Laboratories and government agencies such as NRC and DOE. The NROP fellows would conduct numerical and experimental investigations of thermal-hydraulics problems relevant to the design, operation and safety of current and future nuclear reactors. They will be American citizens or permanent residents from under-represented minority groups and selected based on their past academic performance, interests and motivation to pursue careers in the nuclear field.

The aims and objectives of this program have not changed from those initially approved by NRC.

II. Progress and Results

Graduate Fellowships

Two M.Eng. students, Mr. Debbrata DÈand Mr. Jorge PÈ and one Ph.D. student, Mr. Kalu UÈhave received NY-NROP fellowships starting in 2011. The fellowships are worth \$16,000 per year in stipend for M.Eng. students and \$30,000 per year for a Ph.D. student, plus tuition fees and health insurance.

Mr. Debbrata DÈ the first M.Eng. student who was selected to receive an NROP fellowship, has been conducting experimental research on subcooled flow boiling since January, 2011, in the Nuclear Thermal-hydraulics and Safety Research Laboratory in connection with DOE's Nuclear Simulation HUB Project, CASL. He has been successfully conducting air bubble injection experiments under guidance from Prof. M. Kawaji and his experimental results will be included in an M.Eng. thesis to be completed by the end of May, 2012 as well as a conference paper for submission by May 7, 2012. He has also received a full-time job offer from the Naval Air Systems and also a job interview at Nuclear Regulatory Commission. He will graduate at the end of May and begin his work as a full time engineer shortly afterwards.

Mr. Jorge PÈ started his M.Eng. program in Mechanical Engineering in September, 2010, and received an NROP fellowship in September, 2011. He has been conducting research on thermal energy storage based on thermochemical reactions for use with high temperature nuclear reactors advised by Prof. M. Kawaji. He presented a paper entitled "Thermochemical Heat Storage System for High Temperature Nuclear Reactors and Solar Thermal Power Plants" at the International Conference of Alternative Energy 2011 in San Juan, Puerto Rico, October 3-4, 2011. He has started applying to engineering jobs as he is expected to successfully complete his M.Eng. thesis and graduate at the end of May, 2012. Mr. Sæř ÁWÈstarted his Ph.D. program in September, 2008, and has been advised by Prof. Taehun LÈ to conduct research on numerical simulation of reactor thermalhydraulics problems using a Lattice Boltzmann model. Mr. Sæř ÁJÈ received the NROP fellowship in September, 2011, and has made progress as described in the appendix.

Meetings with Nuclear Experts

All NROP Fellowship students had an opportunity to attend the following seminars and meet with the nuclear experts who were invited to visit CCNY.

Dr. James C. Higgins of Brookhaven National Laboratory gave a talk entitled "Importance of Human Performance to Safety in Complex Industries" on October 14, 2011.

Dr. Hossein Nourbakhsh from US NRC gave a talk entitled "Reactor Safety Regulations and New Reactor Licensing Process" on September 28, 2011 and "Dealing with Uncertainties in Reactor Safety Decisions" on October 28, 2011.

Dr. Eric Loewen, President of ANS, visited CCNY on October 13, 2011, gave two seminar talks entitled "Fukushima and Role of Past severe Accident Research", and "The American Nuclear Society President's Special Committee on Used Nuclear Fuel Management Options".

Prof. Bal Raj Sehgal of Royal Institute of Technology in Sweden gave a talk entitled "Light Water Reactor Safety: History, Accidents and Safety Research", on November 4, 2011.

Dr. Nick Simos of Brookhaven National Laboratory gave a talk entitled "Nuclear Reactors and Seismic Design Considerations. An Overview" on December 2, 2011.

Mr. Alphonse Aliperti (VP Engineering) and Samuel W. Petrosi (Chief Nuclear Engineer) from Burns & Roe gave a talk on their nuclear engineering business on March 22, 2012.

Dr. Marianne Francois from Los Alamos national laboratory gave a guest lecture on numerical simulations of multiphase system using an interface tracking method on March 22, 2012.

Recruitment

To recruit students from under-represented minority groups, flyers describing the NY-NROP Fellowship and other fellowships available at City College of New York for graduate studies in nuclear engineering were sent to 40 Nuclear Engineering Departments in the US. Also, the same information was added to the CUNY Energy Institute's website at http://energy.cuny.edu/energy/about/Nuclear.html

Following our multiple visits to the University of Puerto Rico's Mayaguez (UPRM) campus in 2010 and 2011 for recruitment, one Master's student has applied for admission into our Ph.D. program in Fall, 2012. He was subsequently awarded a CCNY Graduate Fellowship in the first year of his PhD study. He will be eligible for an NROP Fellowship starting in Fall, 2013.

III. Significance

This project has had a successful start by finding well qualified students from underrepresented minority groups, e.g., African American and Hispanic groups, who are well motivated to pursue a career in nuclear engineering upon completion of their M.Eng. and Ph.D. degree programs.

IV. Plans

As two M.Eng. students will be graduating in May, 2012, we will recruit one more graduate student for the NY-NROP fellowship program in September, 2012.

 A comparison of actual accomplishments with the goals and objectives established for the period.

Three recipients of the NY-NROP Fellowships have been found for the academic year 2010-11 and 2011-12 as originally planned. The fellowship students have been pursuing a nuclear engineering-related study and conducting research work in the nuclear reactor thermal-hydraulics area. One of the two M. Eng. students soon to graduate has received full-time job offers to join the nuclear workforce.

Progress report for the period of September 2011 to March 2012

Name: Kalu U0 Mentor: Dr. Taehun L.

Project : SEDG-LBM / NEKLBM

My research interest is in high order simulations using the Lattice Boltzmann equation and Spectral Element Discontinuous Galerkin (SEDG) approach. I am working on the NEKLBM code which has been developed by Dr. Taehun L. and Dr. Misun M. in collaboration with Dr. Paul Fischer at Argonne National Laboratory.

External Forcing with Lattice Boltzmann Method

So far the NEKLBM code can only be used to solve laminar flows. There are papers published by Dr. Taehun L., Dr. M. and Kalu U. that shows how well the results from SEDG Lattice Boltzmann model compares to results from other literatures. Our results show exponential convergence with increasing polynomial order.

My approach to using NEKLBM to test turbulent simulation in a pipe is to first solve the two dimensional channel flow problem with constant pressure gradient, and then proceed to pressure driven flow in a channel. After these results are verified, I will proceed to collecting turbulence simulation statistics in a pipe.

An external forcing term which will drive the flow has been added to the Lattice Boltzmann equation (LBE) and implemented in the NEKLBM code. This addition led to the formulation of a new collision equation for the lattice Boltzmann model. The new Lattice Boltzmann formulation with the collision and streaming steps are shown below.

COLLISION :

$$\overline{f_{\alpha}}(x,t) = \overline{f_{\alpha}}(x,t) - \frac{1}{\tau + 1/2} (\overline{f_{\alpha}} - \overline{f_{\alpha}^{eq}})\Big|_{(x,t)} + \delta t \left(\frac{e_{\alpha} - u}{\rho c_{s}^{2}}\right) \frac{(P_{L} - P_{0})}{L} \bullet f_{\alpha}^{eq}\Big|_{(x,t)}$$

STREAMING :

$$\frac{\partial \overline{f_{\alpha}}}{\partial t} + e_{\alpha i} \frac{\partial \overline{f_{\alpha}}}{\partial x_i} = 0$$

Where $\overline{f_{\alpha}}$ is the particle distribution function and the last term in the collision equation is the contribution from external forcing. The streaming step is the advection equation. This formulation has been tested for 2D plane channel, 3D rectangular channel, and 3D circular channel.

2D plane Channel

In this test a constant pressure gradient (external forcing) was applied in the x-direction with an initial zero velocity everywhere in the channel. The top and bottom boundaries have zero velocity. Periodic boundary condition was imposed at inlet and outlet. The Reynolds number for this simulation is 100, the total number of elements is 96, the order of the spectral interpolating polynomial is 5, and the Courant number is 0.4. The channel height is 1, and the length of the channel is 10. The numerical solution was compared with the exact transient solution of this

problem. The solution for the velocity in the x-direction begins to match after about 60 iterations and the steady state result shows an error of order 10^{-6} . A plot of the velocity profile for the exact solution and numerical computation is shown in the figure 1.

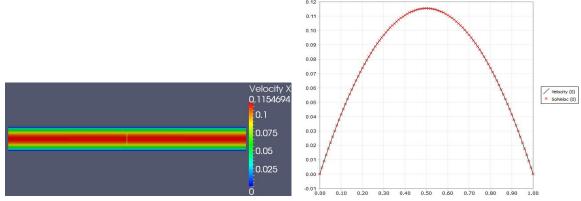


Figure 1, Steady state velocity profile for channel flow

Figures 2 and 3 show the plot of average velocity and average shear stress in the channel with time respectively.

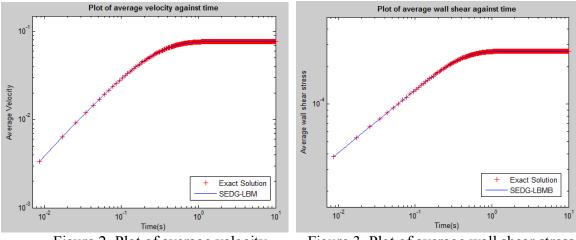


Figure 2, Plot of average velocity

Figure 3, Plot of average wall shear stress

The results show that NEKLBM solutions are in good agreement with the exact solution.

3D pipe flow

In this test a constant pressure gradient was applied in the z-direction with an initial zero velocity in the channel. The Reynolds number for this simulation is 100 and the Courant number is 0.4. The pipe diameter is 1, and the length of the pipe is 10. The numerical solution was compared to the exact transient solution of this problem. Figure 4 shows the geometry of the pipe. A plot of the velocity profile for the exact solution and numerical computation is shown in the figure 5.

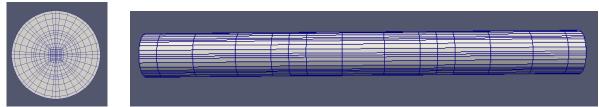


Figure 4, Pipe Geometry: 60 elements, 20 elements on xy plane. 8 elements on the circumference

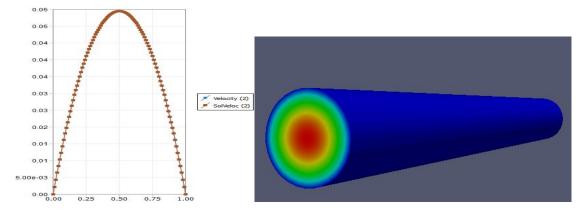


Figure 5, Velocity profile of pipe flow at steadt state

Direct numerical simulation of freely decaying turbulence

The SEDG Lattice Boltzmann discretization is used to study the time evolution of a three dimensional (3D) high-symmetry initial condition. This flow has been studied by Kida (1985), Kida & Murakami (1987), Boratav & Pelz (1994), and others.

Some examples of flows with highly symmetric initial condition are the Taylor-Green vortex flow and the well known kida vortex flow. These flows have been extensively studied within a domain with periodic boundary conditions. For this study, simulations are carried out in a cube of dimension $\in [0, 2\pi]$. The meshes considered are 20³ and 32³ respectively. The order of the interpolating polynomial, N is varied from 5 to 10. Thus, for a 32³ simulation and N = 8, the number of node points is 2573.

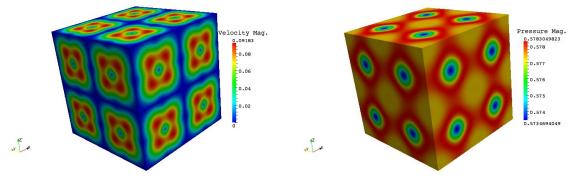
The Initial condition for the kida vortex flow is;

$$u_x(x, y, z, t = 0) = U_0 \sin x(\cos 3y \cos z - \cos y \cos 3z)$$

$$u_y(x, y, z, t = 0) = U_0 \sin y(\cos 3z \cos x - \cos z \cos 3x)$$

$$u_z(x, y, z, t=0) = U_0 \sin z (\cos 3x \cos y - \cos x \cos 3y)$$

where x, y, and $z \in [0, 2\pi]$, and periodic boundary condition is applied. In the Lattice Boltzmann (LB) framework, the Reynolds number is Re = 4000, and the average velocity is $u_0 = 0.05$ which corresponds to a Mach number, Ma, of 0.0866. The D3Q19 (3-dimensional, 19 velocity) model is used to perform the LB simulation. In order to get symmetric initial pressure for the Kida vortex simulation, the code was ran without updating the velocity field for a very long time until the pressure becomes symmetric. The initial condition and symmetric pressure are shown in figure 6 and figure 7 respectively.



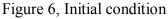


Figure 7, Symmetric pressure after 100000 iterations

Kinetic energy and enstrophy are two important global quantities that characterize the history of the flow. The initial iso-surface of the vorticity magnitude is shown in figure 8. Plots of the kinetic energy and enstrophy are shown in figures 9 and 10 respectively for N = 5 and mesh dimension of 20^3 . To fully resolve this decaying turbulence flow a finer mesh and larger computer memory is required. This job is being moved to the clusters of the City University of New York High performance Computing Center (CUNY-HPC) where memory allocation will not be an issue.

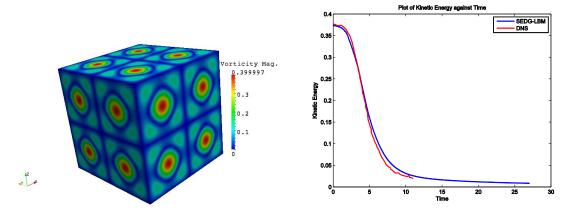


Figure 8, Iso-Surface of Vorticity

Figure 9, Plot of Kinetic Energy

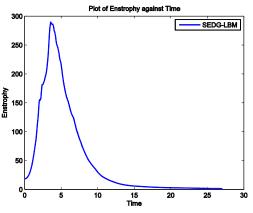


Figure 10, Plot of enstrophy