Imperial College London

Department of Earth Science and Engineering

MSc in {Applied computational science and engineering}

Independent Research Project

Project Plan

Parallelisation of the iSALE shock physics code using a hybrid OpenMP/MPI approach

by

Mohan Sun

Email: mohan.sun21@imperial.ac.uk

GitHub username: ms921

Repository: https://github.com/ese-msc-2021/irp-ms921

Supervisors:

Professor Gareth S. Collins

Dr. Tom Davison

July 2022

Abstract

Impact activity has enormous effects on the formation of the solar system and human life. Therefore, exploring impact activities is an important field in earth science. iSALE is a world-class tool developed for simulating impact events and investigating the effects of various parameters based on Lagrangian Eulerian. This project aims to improve the functionality and realize parallelization of current iSALE hydrocode. In this report, relevant background and algorithm of iSALE will be introduced. Project objectives will be described in detail. In addition, the current progress and future plan will be provided.

Content

1. Introduction 4

2. Literature Review 4

2.1 Fundamental equations of iSALE 4

2.2 Resolution 5

2.3 iSALE-3D workflow 6

3. Problem Description and Objectives 7

4. Progress to Date and Future Plan 8

5. Bibliography 9

Appendix : Gantt Chart 10

1. Introduction

Investigating the impact-related processes is a significant part in planetary science to help people learn about the evolution of many planets such as the formation of craters on the surface of the moon. In addition, impact processes can bring both favorable and unfavorable effects on human life[1]. For example, it is considered that the major extinction event that happened at the Cretaceous – Paleogene boundary is closely related to a devastating impact[2]. On the other hand, a number of important deposits were formed from impact activities[1]. Nevertheless, the complex large-scale impact processes are generally high-cost and difficult to be simulated in the laboratory. Furthermore, the enormous energy generated by the impact event is difficult to control by the experimenters.Therefore, numerical modelling becomes a powerful technique for researching cratering events and investigating the effects of different physical parameters[3]. A problem followed by the rise of numerical simulation is accuracy. At the early stage of impact modelling, because of the limitations of computer hardware, researchers regarded models as vertical impact and simplified the models to two dimensions based on the symmetry of the impact processes[3]. However, actually the phenomenon of vertical impact is almost non-existent in reality, and the study found that the most common impact angle should be 45 degrees[4].

In 1980, a Simplified Arbitrary Lagrangian-Eulerian(SALE) hydrocode was designed to calculate two-dimensional fluid flows at all speeds[5]. Based on the original SALE code, a multi-material, multi-rheology shock physics code impact-SALE(iSALE) was developed to enhance, correct and extend features of SALE[6]. iSALE is a effective tool for impact study, and currently it has been applied for investigating the mobility of large rock avalanches, the formation of large impact craters on planets, effects of water layer to formation of craters, and influences of various parameters on crater formation[7]. Till now, the iSALE hydrocode is still under development. Since complicated calculations are processed and a large number of timestamps can be required during 3-D impact modelling, parallelisation could be a powerful technique to improve the computational efficiency of the hydrocode. In addition, as different models have different sensitivities to resolution, and resolution is closely linked to the time cost computation cost of the code, regriddinging becomes a essential part to find a suitable resolution for the model.

This project would mainly work on learning about the algorithm and principles involved in iSALE3D hydrocode. Additionally, regridding function in iSALE3D will be implemented. Furthermore, parallelisation of regridding function is going to be realized using hybrid OpenMP and MPI approach.

2. Literature Review

2.1 Fundamental equations of iSALE

Since the materials involved used in the impact process (e.g. most fluids, solids) are much larger than atoms on the smallest scale, the macroscopic medium can be viewed as a continuum of tiny materials based on the scale separation between macroscopic and microscopic behavior, to better describe the macroscopic behavior of the material during impact process[8]. Therefore, the dynamics of a continuous material can be expresses by the differential equations of conservation of mass, energy, momentum. Depending on the observer’s frame of reference, the three equations can be expressed in two forms: Lagrangian description and Eulerian description[9].

Lagrangian description of conversation laws is applied to the reference frame that follows the moving parcels:

Conservation of Mass: $$\frac{D\rho}{Dt} = -\rho \frac{\partial v_i}{\partial x_i}$$

Conservation of Momentum: $$\rho \frac{Dv_i}{Dt} = c_i + \frac{\partial \sigma_{ji}}{\partial x_j}$$

Conservation of Energy: $$\frac{DW}{Dt} = -\frac{p}{\rho}\frac{\partial v_i}{\partial x_i} + s_{ij}\dot{\epsilon}'_{ij}$$

Eulerian description of conversation laws is applied to the reference frame that focuses on a specific location in space:

Conservation of Mass: $$\frac{\partial \rho}{\partial t} + v_i \frac{\partial \rho}{\partial x_i} = -\rho \frac{\partial v_i}{\partial x_i}$$

Conservation of Momentum: $$\rho \frac{\partial u_i}{\partial t} = c_i + \frac{\partial \sigma_{ji}}{\partial x_j}$$

Conservation of Energy: $$\rho \frac{\partial W}{\partial t} = -p \frac{\partial v_i}{\partial x_i} + s_{ij}\dot{\epsilon}'_{ij}$$

Where v_i is the velocity, ρ is the material density, c_i is the external force to material per unit mass, σ_{ji} is the stress tensor, W is the specific internal energy, s_{ij} is the deviatoric stress tensor, and $\dot{\epsilon}'_{ij}$ is the deviatoric strain rate[3].

The Lagrangian reference frame is employed when the observer investigate the path of particles in the fluid, the Eulerian reference frame is applied when the observer inspect a certain area and observe particles passing through this area. The algorithm involved in iSALE attempts to solve equations of conservation laws in an arbitrary reference frame, which means the system of equations are firstly solved in a Lagrangian reference frame and then translated into a different reference frame if required, which is the Arbitrary Lagrangian Eulerian(ALE) solution[10].

2.2 Resolution

In impact model, the number of computational cells per prjectile radius(CPPR) is generally used to represent the resolution[3](shown in Figure 1). Since the materials are represented by a finite number of cells, as the number of cells(resolution) increases, the error will be reduced. Nevertheless, higher resolution can lead to higher computational cost, higher memory cost, and longer calculation time[3]. In addition, the resolution requirement of impact models depends on the problem to be solved. For instance, studies shows that material experiencing a certain peak pressure is relatively more sensitive to resolution than diameter ted and crater depth[11][12]. Therefore, resolution test is significant in numerical impact modelling.

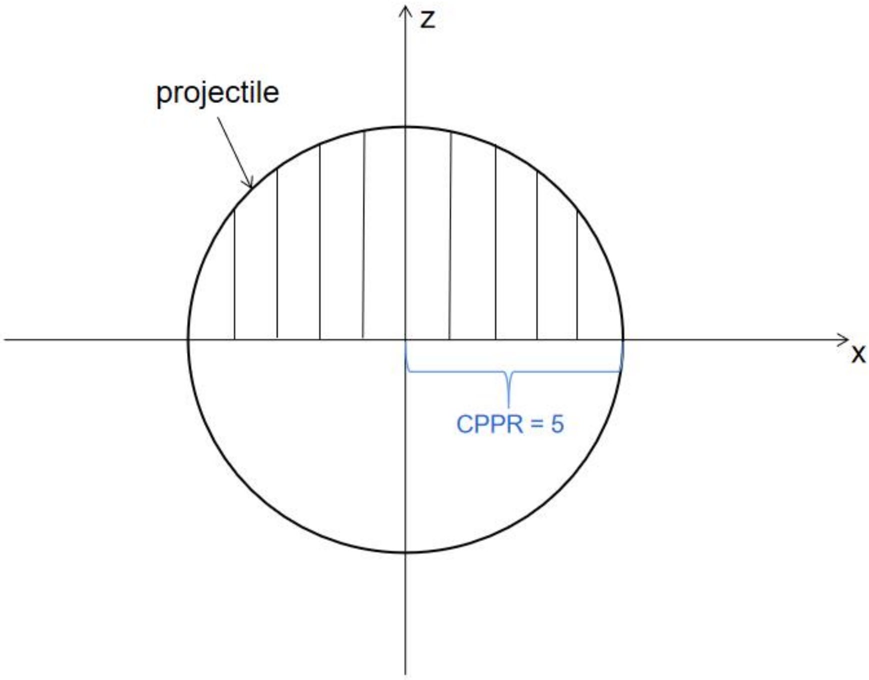

Figure 1: Projectile and Cells Per Projectile Radius(CPPR).

2.3 iSALE-3D workflow

The algorithm of iSALE3D hydrocode is basically divided into four parts, which are problem setup, cycle advance, Lagrangian step, and cycle completion[13](as shown in Figure 2). For iSALE3D, since MPI/OpenMP is applied, domain decomposition is required at the beginning of the program to divide domains into several sub-domains by splitting the mesh at regular intervals in the x-direction. During the stage of problem setup, a model is initialized or restored from a previous model. The assignment of material parameters, allocation of memory space and generation of mesh are completed. After that, the cycles are started. At the initial stage of a cycle, cell-centered variables(such as pressure, density, etc.) are updated and tracer particles move in the mesh. Then during the Lagrangian step, the effect of all forces to the velocity field and variation of internal energy are computed and updated. At the final stage of a cycle(Advection), the face fluxes and relevant field quantities are calculated, then the velocity vector filed is advected by defining and conservatively transporting cell-centric momentum between cells[13].

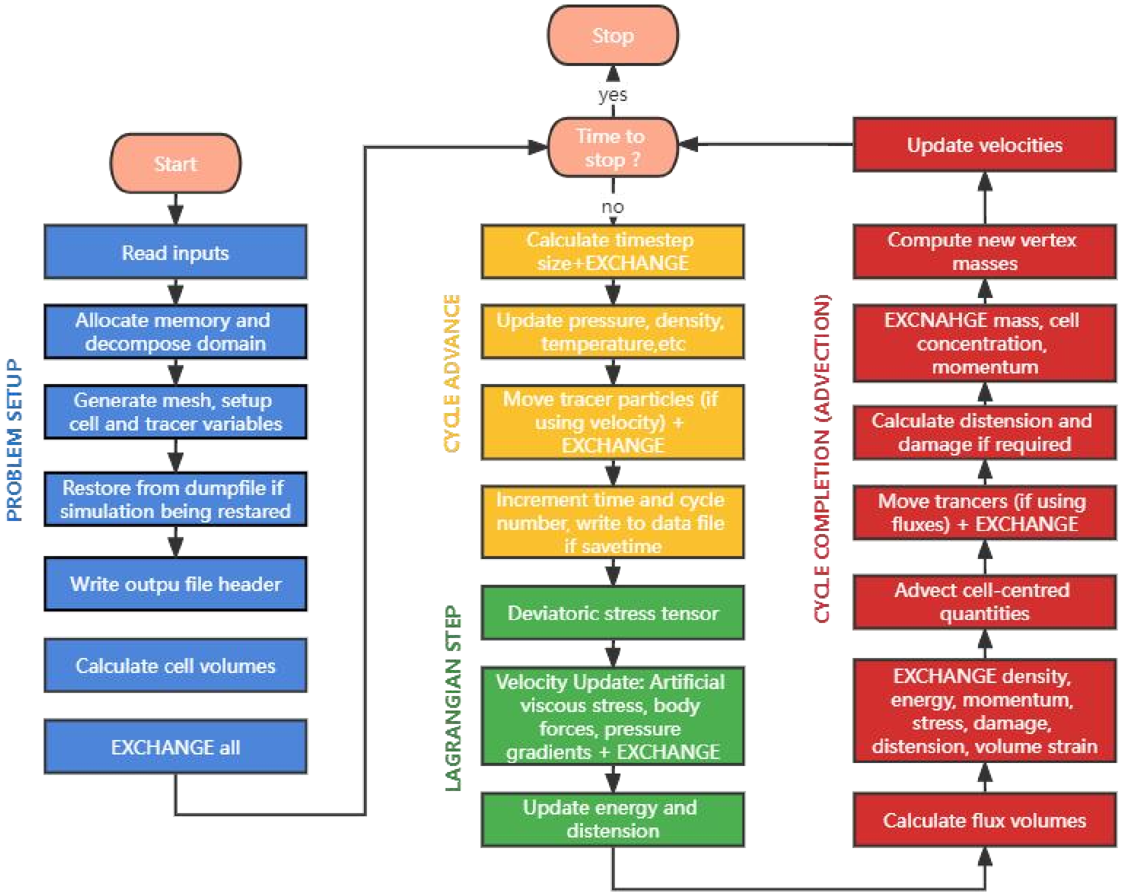

Figure 2: iSALE-3D workflow diagram.

3. Problem Description and Objectives

This project aims to improve the efficiency of iSALE3D code while ensure the high accuracy of solutions. In this project, there are three types of regridding strategies to be implemented.

- For the first method, the physical space is kept unchanged and the resolution is going to be reduced, so the number of cells in the physical space will decrease by combining multiple cells into one cell. For example, in iSALE-2D, 4 cells are gathered into one, while in iSALE-3D, 8 cells might be gathered into one.

- For the second method, the physical space is expanded without changing the number of cells, hence the size of each cell is going to be increased and as a consequence resolution is reduced.

- For the third method, the range of the physical space is expanded without modifying the resolution, therefore, more cells is going to be added in the field.

Furthermore, MPI/OpenMP approach is going to be included during the development of three regridding methods. After that, the performance test will be adopted to check the efficiency and accuracy of the code.

4. Progress to Date and Future Plan

Till now, the Linux system and related configuration have been completed. iSALE has been successfully run in the Linux system with MPI. In addition, a python script which plots the restored model and old model was developed to verify that the model was successfully inherited from dump file. For the future plan, a Gantt Chart was created to show the timeline more intuitively(shown in Appendix).

5. Bibliography

[1] Pati, J.K. and Reimold, W.U. (2007). Impact cratering — fundamental process in geoscience and planetary science. *Journal of Earth System Science.* 116, pp. 81–98.

[2] Smit, J. and Hertogen, J.(1980). An extraterrestrial event at the Cretaceous–Tertiary boundary. *Nature,* 285 198–200.

[3] Collins, G., Wuennemann, K., Artemieva, N., and Pierazzo, E. (2012). Numerical modelling of impact processes. *In Impact Cratering: Processes and Products*, pp. 254–270. Wiley-Blackwell.

[4] Pierazzo, E. and Melosh, H.J. (2000) Understanding oblique impacts from experiments, observations, and modeling. *Annual Reviews in Earth and Planetary Science*, 28, pp.141–167.

[5] Amsden, A., Ruppel, H., and Hirt, C.(1980) SALE: A simplified ALE computer program for fluid flow at all speeds. *Los Alamos Scientific Lab.*, Los Alamos, New Mexico: LANL, Rep. LA-8095.

[6] Collins, G. S., Elbeshausen, D., Wünnemann, K., Davison, T. M., Ivanov, B., and Melosh, H. J.(2016). iSALE-Dellen manual: A multi-material, multi-rheology shock physics code for simulating impact phenomena in two and three dimensions. dx.doi.org/10.6084/m9.figshare.3473690.

[7] iSALE. Available: https://isale-code.github.io.

[8] Robert H. C. Moir. Introduction and Overview of Hydrocodes for Impact Cratering Modeling[Online]. *Western University.* Available:http://phenomenologica.com/docs/expositions/Introduction%20and%20Overview%20of%20Hydrocode%20for%20Impact%20Cratering%20Modeling.pdf.

[9] Malvern, L.E. (1969) An Introduction to the Mechanics of a Continuous Medium, Prentice-Hall, Englewood Cliffs, New Jersey.

[10] Benson, D. J. (1992). Computational methods in lagrangian and eulerian hydrocodes. *Computer methods in applied mechanics and engineering*, 99(2-3):235.

[11] Pierazzo, E., Vickery, A.M. and Melosh, H.J. (1997) A reevaluation of impact melt production. *Icarus*, 127, pp.408–423.

[12] Wünnemann, K., Collins, G.S. and Osinski, G.R. (2008) Numerical modelling of impact melt production in porous rocks. *Earth and Planetary Science Letters*, 269 (3–4), pp.530–539.

[13] Collins, G. S., Elbeshausen, D., Wünnemann, K., Davison, T. M., Ivanov, B., and Melosh, H. J(2022). iSALE: A multi-material, multi-rheology shock physics code for simulating impact phenomena in two and three dimensions.

Appendix : Gantt Chart