Science and Technology Facilities Council

WP2 of CCP-NTH

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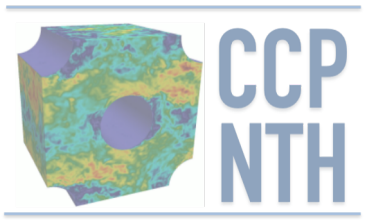
The second Management Committee Meeting (MCM) for CCP-NTH
20th January 2021



Overview of WP2: Code Development and maintenance

WP2-0 Project management and website/database maintenance

WP2-1 Robust CFD

WP2-2 High fidelity simulations using DNS/LES

WP2-3 Technical support

WP2-0 Project management and website/database maintenance

Website:

- Website is not yet available due to the updating of web severs for CoSeC CCP/HEC.
- CoSeC is working on unifying website schemes with a new content management system (CMS) for all CCPs as the current default CMS Drupal 7 will come to end of life by June 2021. Several CoSeC CCP/HEC Website Working Group Meetings have been carried out (13th Oct, 20th Oct, 05th Jan).
- The website (www.ccpnth.ac.uk) will be built with support teams from System Division (STFC) once the selected CMS Wordpress is installed in the new server.
- Current news & events:
  - https://www.scd.stfc.ac.uk/Pages/CoSeC.aspx
  - https://twitter.com/CoSeC_community

WP2-1 Robust CFD

WP2.1.1 Coarse Grid CFD:

- **Objective:** to validate the coarse-grid scheme, Sub-Channel CFD, developed in the project of Digital Reactor R&D (BEIS); to potentially make SubChCFD a robust Code_Saturne add-on module
- **Some updates on SubChCFD activities (from UoS , UoM, EDF Energy)**
  - Coupling with resolved CFD and porous modelling have been developed through BEIS Digital Reactor Design –TH project;
  - Some investigation/discussion are being made to consider potential integration of SubChCFD to Nuclear Virtual Engineering Capability (NVEC), another BEIS NIP project;
  - A new PhD has started at Sheffield to work on transient SubChCFD.

WP2-1 Robust CFD

Performance of *Code_Saturne* in Archer2:

- *Code_Saturne's* performance has been tested during ARCHER2 early access. It is consistently **four times faster** on one Archer2 node (128 cores) than that on one Archer node (24 cores) using the same test case.

New Project:

- Charles Moulinec and Wei Wang of STFC's Computational Engineering Group together with Co-investigators Shuisheng He and Bo Liu (University of Sheffield) and collaborator Juan Uribe (EDF), have been successful with the ARCHER2 Pioneer proposal "High-Fidelity Simulations to Improve Performance and Safety of PWRs". A very detailed LES of a "ballooning" situation will be carried out using *Code_Saturne* in Archer2.

WP2-2 High fidelity simulations using DNS/LES

CHAPSim1.0

- release of the first unified CHAPSim code after collecting, comparing and merging different versions from different research groups. (CHAPSim1.0)
- Github repo for CHAPSim1.0: https://github.com/WeiWangSTFC/CHAPSim
  - *Please contact me if anyone of your groups is interested in using CHAPSim for their research.*

Main features of CHAPSim1.0

	Methods
Parallel	MPI
Mesh	Structured, generated on the fly
Spacial Discretization	Finite Difference
Nonlinear terms	Divergence form
	2nd order spacial accuracy
	explicit Runge-Kutta & Adams-Bashforth method for temporal discretization
Viscous terms	implicit Crank-Nicolson method for temporal discretization
Pressure	FFT and Fractional step method
Thermodynamics	Quasi-incompressible flow
	Thermal properties updated by table-searching or specified functions of temperature

Directory structures of CHAPSim1.0

bin	1 item	Folder	2020-10-27 15:45:41
docs	3 items	Folder	2020-10-21 16:57:44
lib	3 items	Folder	2020-10-15 10:44:27
obj	140 items	Folder	2020-10-27 15:45:41
scripts	13 items	Folder	2020-10-15 10:44:27
src	66 items	Folder	2020-11-04 01:02:10
test_cases	18 items	Folder	2020-10-19 10:46:32
test_cases_additional	10 items	Folder	2020-10-19 10:46:15
test_cases_template	17 items	Folder	2020-10-19 10:59:01
test_loop	2 items	Folder	2020-10-15 10:44:27
.git	12 items	Folder	2020-10-28 08:36:28
.vscode	1 item	Folder	2020-10-20 09:48:04
CHAPSim_workspace.code-workspace	60 bytes	Unknown	2020-10-22 20:54:37
LICENSE	35.1 kB	Text	2020-10-16 09:08:58
Makefile	6.5 kB	Text	2020-10-27 14:39:54
README.md	3.6 kB	Text	2020-10-26 16:46:50
.gitignore	394 bytes	Text	2020-10-23 14:38:02

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CoSeC Computational Science Centre for Research Communities

WP2-2 High fidelity simulations using DNS/LES

CHAPSim1.0 – *further work done after the initial unified version*

- **I/O:**
  - formatting/cleaning CHAPSim with new user-friendly input and output interfaces, to make the code more accessible
  - Working with users (from Liverpool John Moores University) to improve/optimise the postprocessing in the code, mainly for ensemble and phase averaging in the case of pulsating flows
- **Precision:** Updating the Fishpack FFT library to double precision to improve its portability
- **Functions added and tested:**
  - Added functions to deal with liquid metals (ie. liquid sodium, liquid lead, liquid bismuth and liquid LBE) to expand its application to unique media for advanced nuclear reactors
  - Added functions to deal with liquid water at subcritical condition to support the projects in the LJM university
  - Developed a conjugate heat transfer module in collaboration with Sheffield group, now included in a test version. The latest version of CHAPSim has been distributed to the main users for testing its application in their specific domains.

WP2-2 High fidelity simulations using DNS/LES

CHAPSim1.0 – *further work done after the initial unified version*

- Code Performance:
  - Assessing the performance of CHAPSim1.0 on Archer2: good scaling until 10*128 cores (10 nodes), with the scaling levelling after that; out of memory issues for big meshes (eg. 34M cells for 2 nodes (2*128 cores). These will be corrected in CHAPSim2.0.
- Docs:
  - Writing an ”Introduction to CHAPSim” available to download in https://github.com/WeiWangSTFC/CHAPSim
  - Slides about the code performance
- Users Meeting:
  - A high-level python data postprocessing and visualization tool has been developed in Sheffield Group and made available via current CHAPSim users.

WP2-2 High fidelity simulations using DNS/LES

CHAPSim2.0

- **Main aims:**
  - multi-dimensional MPI (2D-pencils) + high order accuracy
  - Fast calculation and high HPC performance.
- **Initial plans:** based on the CHAPSim1.0; firstly, multi-dimensional MPI; then high order accuracy
- **Changed plans:** from scratch. Multi-dimensional MPI and high order accuracy implemented at the same time
  - After analysing the features of explicit central difference high-order and compact higher order FD, **the compact scheme for FD** is adopted for the high-order accuracy.
  - For a compact FD scheme, the global variables are required to solve the compact equations, which requires MPI to fetch global variables, rather than only building up the domain interface.

WP2-2 High fidelity simulations using DNS/LES

CHAPSim2.0

- **Why choose compact scheme for high order? Why the MPI is highly related to the FD scheme chosen?**

		Explicit high order	Global compact scheme
Numerical methods	**pros**	- Local calculation of finite difference and interpolation operators. - No TDMA for tri-diagonal eqs solved (except Poisson Eq.). Fast.	- Less nodes required for a stencil - Low dispersion error - Keep high order at boundaries
	cons	- More nodes for a stencil - High dispersion error - Accuracy reduced near non-periodic boundaries	- Require global compact scheme for finite difference and interpolation. - To solve tri-diagonal eqs to get finite difference and interpolation of variables, slow.
Coding	**pros**	- No fetch of global variables. Fast.	
	cons	- Fetch multi-layer information from neighbouring domain.	- Fetch global variables for compact schemes. Slow.
MPI	**interface**	- Fixed. No transpose for NS. Fast - Double transpose for FFT.	- Multiple transpose for NS and FFT.
	To get global information	- MPI_SENDRECV to fetch multi-layer information **from neighbouring domains.** Fast.	- MPI_ALLTOWALL to **distribute variables globally**. Slow.
Examples		Morinishi1998, CHAPSim1.0(2nd)	incompact3d

WP2-2 High fidelity simulations using DNS/LES

CHAPSim2.0

- Literature review about different schemes/techniques to build **the main features** of CHAPSim2.0

Features	Options	Choice
Accuracy order	• 4th • 6th	6th order to capture fine turbulence features caused by variable properties.
Non-uniform mesh	How many directions of non-uniform?	1D non-uniform, wall normal direction 2D uniform mesh, streamwise and spanwise directions
Methods for non-uniform for compact FD	• Coefficient matching from Taylor Expansion • Coordinate transformation	Coordinate transformation with FFT, refer to Cain1984, Laizet2009.
Staggered grids for compact FD	• High order interpolated u, v on nodes and then for (uv), then for d(uv)/dy • High order interpolated u, v on face and then calcuated (uv), and then interpolated (uv) for d(uv)/dy	High order interpolated u, v on nodes and then for (uv), then for d(uv)/dy To reduce operations, to check stability after coding…
Convection term Form	• Divergence form • Skew-symmetric form	Divergence form for staggered mesh to keep local conservation for flows with variable properties.
Temporal Schemes		Flow with constant variable properties: RK - CN Thermal flow: RK

WP2-3 Technical support

- Continue to support CHAPSim Users and Code_Saturne Users
  - Code installing, compiling, debugging for users
  - Answering questions in Users' forum (CHAPSim)
  - Regular Users meetings

WorkPlan

WP2-0 Project management and website/database maintenance

- Continue as normal, visual monthly meeting….
- Work on the website together with CoSeC support

WP2-1 Robust CFD

- Work on the new project in Archer2

WP2-2 High fidelity simulations using DNS/LES

- Work on CHAPSim2.0.
  - To carry on implement and test selected schemes in serial processor
  - To extend to MPI 2D-pencils
  - To test code performance

WP2-3 Technical support

- Continue as normal

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Thank you

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