Science and Technology Facilities Council

CHAPSim2
- beta version release

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**University of Sheffield

CCP/SIG NTH Annual Technical Meeting
27^{th} June 2022

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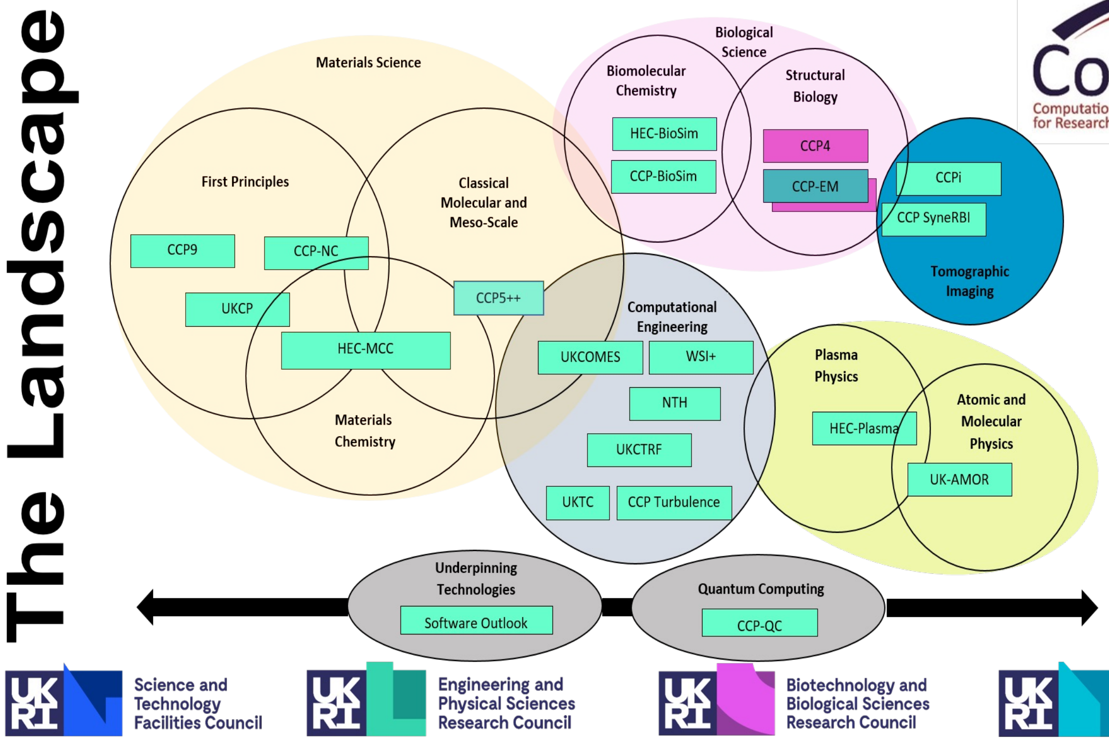


What is CHAPSim?

- *CHAPSim* - A **CH**annel **A**nd **P**ipe flow **sim**ulation solver

CHAPSim77 (2007-2013)

- University of Aberdeen and University of Sheffield
- Dr. Mehdi Seddighi
- Dr. Kui He – cylindrical; Dr. Akshat Mathur – LES
- Fortran 77
- DNS of unsteady turbulence flow in a channel

CHAPSim90-TF (2014-2015)

- University of Sheffield
- Dr. Wei Wang
- Fortran 90
- Incompressible DNS solver for thermo-fluids problems, fluids with strong variation of physical properties

CHAPSim90-TF (2016-2019)

- University of Sheffield, Liverpool Johh Moores, Tsinghua, STFC
- Jundi He – conjugate heat transfer; Matthew Falcone – Boundary layer
- PhD students, RAs
- Application of this solver to fundamental research on turbulence flow, heat transfer and flow development in supercritical CO2/water, fluids to fluids scaling, etc.

CHAPSim1 (2020-2021)

- STFC, University of Sheffield
- Dr. Wei Wang
- Code integration
- Code performance optimisation on ARCHER
- Release of CHAPSim1 in github

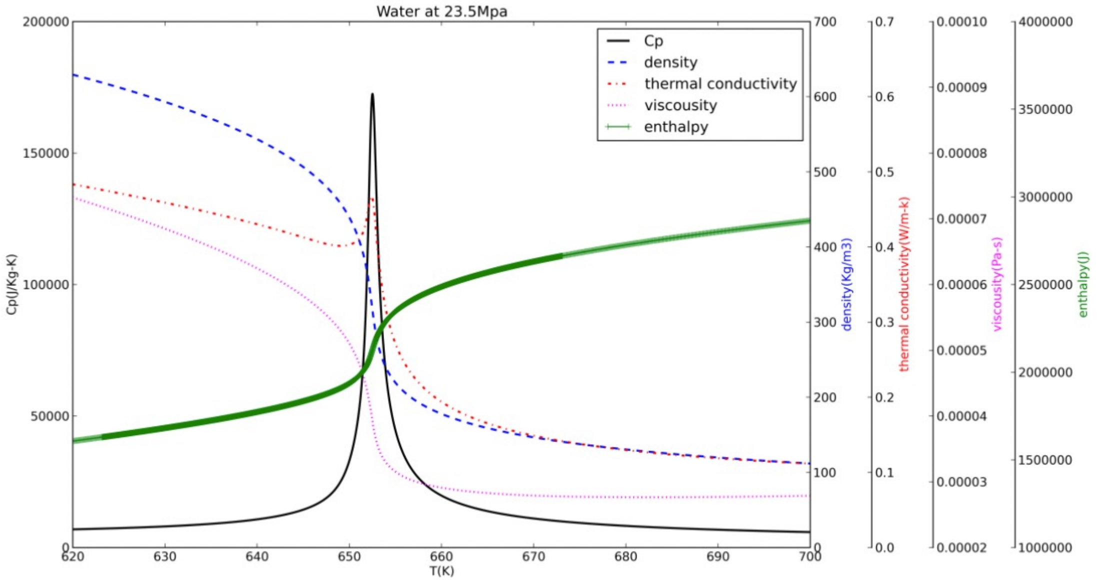
CHAPSim2 (2022)

- STFC, University of Sheffield
- Dr. Wei Wang
- Re-created code structure from scratch
- High-accuracy & high efficient DNS code

Functionalities of CHAPSim

- Physical problems:
  - Incompressible turbulence flow
  - Turbulence flow with the thermal properties varying significantly with temperature but almost independent of the pressure variation. The acoustic interactions and compressibility effects are negligible
  - Heat transfer in the above turbulence flow, forced, natural and mixed convection
  - Conjugate heat transfer
- Fluid media:
  - Fluids at supercritical pressure
  - Liquid metals, sodium, lead, bismuth, lead-bismuth eutectic
- Cases:
  - Channel flow
  - Pipe flow of circular or annular cross-sections
  - Taylor-Green Vortex

- Example 1: water at supercritical pressure



- Example 2: liquid sodium

$$\rho_{Na}[\text{kg m}^{-3}] = 1014 - 0.235 \cdot T$$

$$\ln \eta_{Na}(T) = \frac{556.835}{T} - 0.3958 \cdot \ln T - 6.4406 \quad (\eta \text{ in Pa s})$$

$$c_{p(Na)}(T)[\text{ J kg}^{-1}\text{ K}^{-1}] = -3.001\times10^{6}\cdot T^{-2} + 1658 - 0.8479\cdot T + 4.454\times10^{-4}\cdot T^{2}$$

$$\lambda_{Na}\left[\text{W m}^{-1}\text{ K}^{-1}\right] = 110 - 0.0648\cdot T + 1.16\times10^{-5}\cdot T^{2}$$

Applications of CHAPSim – turbulence

Journal of Fluid Mechanics

Turbulence in transient channel flow

Published online by Cambridge University Press: 09 January 2013

S. He and M. Seddighi

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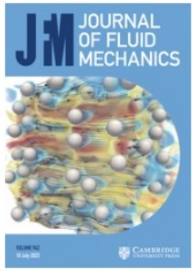
Article contents

Abstract

References



Journal of Fluid Mechanics

Turbulence in a transient channel flow with a wall of pyramid roughness

Published online by Cambridge University Press: 16 September 2015

M. Seddighi, S. He, D. Pokrajac, T. O'Donoghue and A. E. Vardy

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Article contents

Abstract

Introduction

Numerical methods

Geometry, flow conditions and statistical averaging

Results

Conclusions

References

Journal of Fluid Mechanics

Laminarisation of flow at low Reynolds number due to streamwise body force

Published online by Cambridge University Press: 09 November 2016

S. He, K. He and M. Seddighi

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Article contents

Abstract

Introduction

Methodology

Results and discussion

Summary and conclusions

Footnotes

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Abstract

It is well established that when a turbulent flow is subjected to a non-uniform body force, the turbulence may be significantly suppressed in comparison with that of the flow of the same flow rate and hence the flow is said to be laminarised. This is the situation in buoyancy-aided mixed convection when severe heat transfer deterioration may occur. Here we report results of direct numerical simulations of flow with a linear or a step-change profile of body force. In contrast to the conventional view, we show that applying a body force to a turbulent flow while keeping the pressure force unchanged causes little changes to the key characteristics of the turbulence. In particular, the mixing characteristics of the turbulence represented by the turbulent viscosity remain largely unaffected. The so-called flow laminarisation due to a body force is in effect a reduction in the apparent Reynolds number of the flow, based on an apparent friction velocity associated with only the pressure force of the flow (i.e. excluding the contribution of the body force). The new understanding allows the level of the flow 'laminarisation' and when the full laminarisation occurs to be readily predicted. In terms of the near-wall turbulence structure, the numbers of ejections and sweeps are little influenced by the imposition of the body force, whereas the strength of each event may be enhanced if the coverage of the body force extends significantly away from the wall. The streamwise turbulent

- Turbulence flow
  - Transient turbulence flow
  - Turbulence flow laminarisation
  - Spatially accelerating turbulent flow
  - Roughness effect in turbulence transition

Published: 11 March 2011

A Comparative Study of Turbulence in Ramp-Up and Ramp-Down Unsteady Flows

Mehdi Seddighi, Shuisheng He, Paolo Orlandi & Alan E. Vardy

Flow, Turbulence and Combustion 86, 439–454 (2011) | Cite this article

NEAR-WALL BEHAVIOUR OF TRANSIENT FLOW IN A CHANNEL WITH DISTRIBUTED PYRAMID ROUGHNESS

pages 151-156

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Dubravka Pokrajac
School of Engineering University of Aberdeen Aberdeen, UK, AB24 3UE

A Spatially Accelerating Turbulent Flow with Longitudinally Moving Walls

Matthew Falcone & Shuisheng He

Conference paper | First Online: 24 October 2021

204 Accesses

Part of the Springer Proceedings in Physics book series (SPPHY,volume 267)

Applications of CHAPSim – heat transfer

- Heat transfer in flow at supercritical pressure
  - Buoyancy effect
  - Thermophysical property effect
  - Conjugate heat transfer
  - Fluids-to-fluids scaling

Turbulence in a heated pipe at supercritical pressure

Journal of Fluid Mechanics

Published online by Cambridge University Press: 15 June 2021

J. He, R. Tian, P.X. Jiang and S. He

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Article contents

Abstract

References

Direct numerical simulation of convective heat transfer of supercritical pressure CO_2 in a vertical tube with buoyancy and thermal acceleration effects

Journal of Fluid Mechanics

Published online by Cambridge University Press: 29 September 2021

Y.L. Cao, R.N. Xu, J.J. Yan, S. He and P.X. Jiang

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References

ELSEVIER

International Journal of Heat and Fluid Flow

Volume 86, December 2020, 108697

Effects of buoyancy and thermophysical property variations on the flow of supercritical carbon dioxide

Jundi He [a], Junjie Yan [b], Wei Wang [c], Peixue Jiang [b], Shuisheng He [a]

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https://doi.org/10.1

Highlig

- Effects DNS.
- Flow in

ELSEVIER

International Journal of Heat and Mass Transfer

Volume 189, 15 June 2022, 122651

Study of fluid-to-fluid scaling for upward pipe flows of supercritical fluids using direct numerical simulation

Jundi He [a], Wei Wang [b], Junjie Yan [c], Andrea Pucciarelli [d], Peixue Jiang [c], Walter Ambrosini [d], Shuisheng He [a]

The 7th International Symposium on Supercritical Water-Cooled Reactors
ISSCWR-7
15-18 March 2015, Helsinki, Finland

ISSCWR7-1067

Mechanisms of buoyancy effect on heat transfer in a horizontal flow

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Abstract

A complex feature of a heated (or cooled) flow of fluids at a supercritical pressure is that it always continually develops in the flow direction due to the very complex property-temperature relationships, which makes the analysis and data correlation very difficult. We have carried out a fundamental study of flow between parallel plates with heating from one surface and cooling from the other using direct numerical simulation. Under such a condition, the flow can reach a

17th UK Heat Transfer Conference (UKHTC2021)
4-6 April 2022, Manchester, UK

EFFECT OF CONJUGATE HEAT TRANSFER ON THE SIMULATION OF FLOW AT SUPERCRITICAL PRESSURE

Jundi He[1,*], Bing Xu[2], Shuisheng He[1]

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[2]EDF Energy, Barnett Way, Barnwood, Gloucester, UK, GL4 3RS

ABSTRACT

Direct numerical simulations of upward heated pipe flows of supercritical CO_2 at $Re_0 = 3600$ were carried out to investigate the effect of conjugate heat transfer. Simulation results have good agreement in comparison with those from an earlier experiment [1]. It was found that with the solid pipe wall conduction included in the computational model, enthalpy fluctuations close to the wall is largely dampened and wall heat flux is no longer uniformly distributed. Such changes have a minor effect on flow development and turbulence, but they result in some differences in the heat transfer at the early stage of the flow. The Nusselt number (Nu) has a stronger laminar contribution and a weaker turbulent contribution when the thermal conduction of the solid wall is considered, which results in a larger Nu at an early stage but a lower Nu at a later stage compared with the flow case without a solid wall.

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2018, 10-15 August, Beijing, China

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DIRECT NUMERICAL SIMULATION OF CONVECTIVE HEAT TRASFNER IN A VERTICAL PIPE FOR SUPERCRITICAL PRESSURE CO_2

DOI: 10.1615/IHTC16.cms.023324
pages 1753-1760

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Numerical methods –CHAPSim v1 & v2

- Dimensionless incompressible solver
- Finite difference
  - V1: central difference (explicit)
  - V2: compact scheme (implicit)
- Pressure-correction method (Poisson eq)
  - V1: 2-D FFT, periodic bc
  - V2: 3-D FFT, arbitrary bc + 1-D grid stretching
- Conservative variables solved
- Explicit time advancing scheme (RK3)
- MPI Parallelisation
  - V1: 1-D domain decomposition
  - V2: 2-D domain decomposition

Assume

$$
\begin{aligned}
q_1 &= u_1 \qquad g_1 = \rho q_1\\
q_2 &= u_2 \qquad g_2 = \rho q_2\\
q_3 &= u_3 \qquad g_3 = \rho q_3\\
\nabla(\vec{q}) &= \frac{\partial q_1}{\partial x_1} + \frac{\partial q_2}{\partial x_2} + \frac{\partial q_3}{\partial x_3}\\
\nabla^2(u_i) &= \frac{\partial^2 q_i}{\partial x_1^2} + \frac{\partial^2 q_i}{\partial x_2^2} + \frac{\partial^2 q_i}{\partial x_3^2}
\end{aligned}
\tag{4.22}
$$

The continuity equation in conservative form:

$$
\frac{\partial \rho}{\partial t} + \frac{\partial g_1}{\partial x_1} + \frac{\partial g_2}{\partial x_2} + \frac{\partial g_3}{\partial x_3} = 0 \tag{4.23}
$$

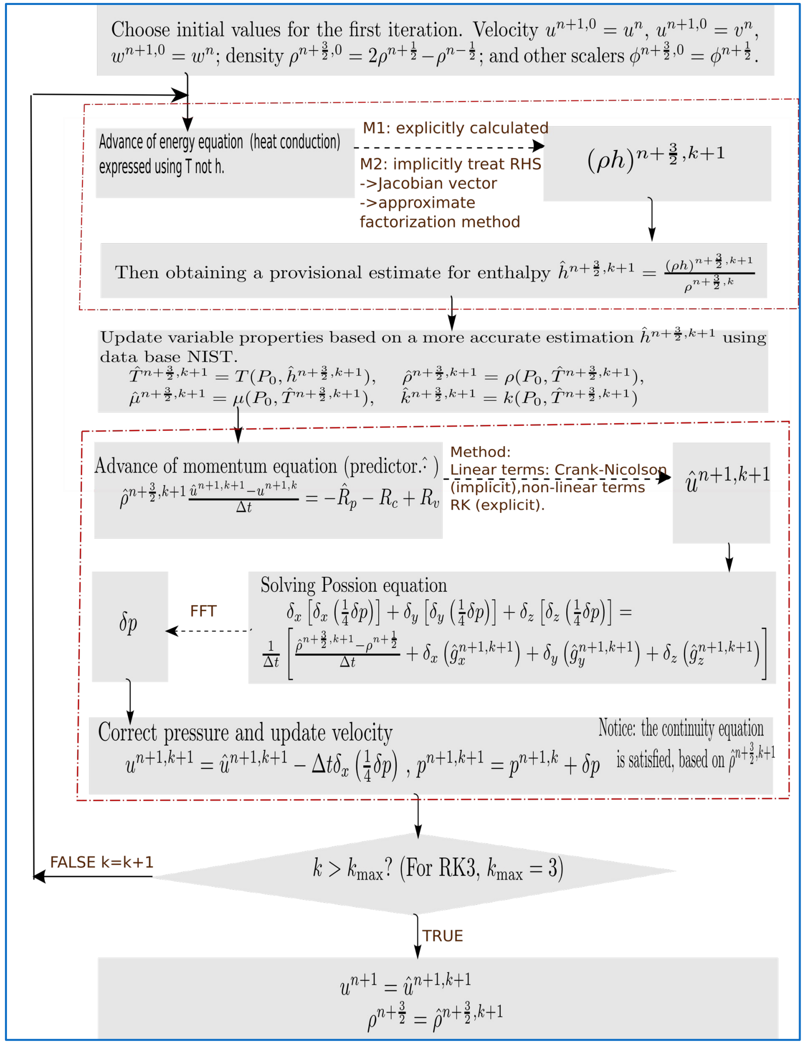
The momentum equation in conservative form:

$$
\begin{aligned}
&\frac{\partial g_1}{\partial t} + \frac{\partial (g_1 q_1)}{\partial x_1} + \frac{\partial (g_2 q_1)}{\partial x_2} + \frac{\partial (g_3 q_1)}{\partial x_3} = -\frac{\partial p}{\partial x_1} + \rho f_1\\
&\mu \cdot \nabla^2(q_1) + \frac{\mu}{3}\frac{\partial(\nabla(\vec{q}))}{\partial x_1} + 2\frac{\partial \mu}{\partial x_1}\cdot\left(\frac{\partial q_1}{\partial x_1} - \frac{1}{3}\nabla(\vec{u})\right) + \frac{\partial \mu}{\partial x_2}\cdot\left(\frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2}\right) + \frac{\partial \mu}{\partial x_3}\cdot\left(\frac{\partial u_3}{\partial x_1} + \frac{\partial u_1}{\partial x_3}\right)\\
&\frac{\partial g_2}{\partial t} + \frac{\partial (g_1 q_2)}{\partial x_1} + \frac{\partial (g_2 q_2)}{\partial x_2} + \frac{\partial (g_3 q_2)}{\partial x_3} = -\frac{\partial p}{\partial x_2} + \rho f_2\\
&\mu \cdot \nabla^2(q_2) + \frac{\mu}{3}\frac{\partial(\nabla(\vec{q}))}{\partial x_2} + 2\frac{\partial \mu}{\partial x_2}\cdot\left(\frac{\partial q_2}{\partial x_2} - \frac{1}{3}\nabla(\vec{u})\right) + \frac{\partial \mu}{\partial x_1}\cdot\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right) + \frac{\partial \mu}{\partial x_3}\cdot\left(\frac{\partial u_3}{\partial x_2} + \frac{\partial u_2}{\partial x_3}\right)\\
&\frac{\partial g_3}{\partial t} + \frac{\partial (g_1 q_3)}{\partial x_1} + \frac{\partial (g_2 q_3)}{\partial x_2} + \frac{\partial (g_3 q_3)}{\partial x_3} = -\frac{\partial p}{\partial x_3} + \rho f_3\\
&\mu \cdot \nabla^2(q_3) + \frac{\mu}{3}\frac{\partial(\nabla(\vec{q}))}{\partial x_3} + 2\frac{\partial \mu}{\partial x_3}\cdot\left(\frac{\partial q_3}{\partial x_3} - \frac{1}{3}\nabla(\vec{u})\right) + \frac{\partial \mu}{\partial x_1}\cdot\left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right) + \frac{\partial \mu}{\partial x_2}\cdot\left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right)
\end{aligned}
\tag{4.24}
$$

The energy equation in conservative form:

$$
\begin{aligned}
&\frac{\partial (\rho h)}{\partial t} + \frac{\partial (g_1 h)}{\partial x_1} + \frac{\partial (g_2 h)}{\partial x_2} + \frac{\partial (g_3 h)}{\partial x_3} =\\
&\kappa \nabla^2(T) + \frac{\partial \kappa}{\partial x_1}\cdot\frac{\partial T}{\partial x_1} + \frac{\partial \kappa}{\partial x_2}\cdot\frac{\partial T}{\partial x_2} + \frac{\partial \kappa}{\partial x_3}\cdot\frac{\partial T}{\partial x_3}
\end{aligned}
\tag{4.25}
$$

$$
\begin{aligned}
\hat{u}_i &= u_i^n + \Delta t\left(\gamma_1 H_i^n + \zeta_1 H_i^{n-1} + \frac{\alpha_1}{2Re} L_{jj}(\hat{u}_i + u_i^n) - \alpha_1 (G_i(p'^n) + S_i^n)\right),\\
L_{jj}(\phi^a) &= \frac{1}{\alpha_1 \Delta t} D_i(\hat{u}_i),\\
\frac{u_i^a - \hat{u}_i}{\Delta t} &= -\alpha_1 G_i(\phi^a),\\
p^a &= p^n + \phi^a - \frac{\alpha_1 \Delta t}{2Re} L_{jj}(\phi^a);
\end{aligned}
$$



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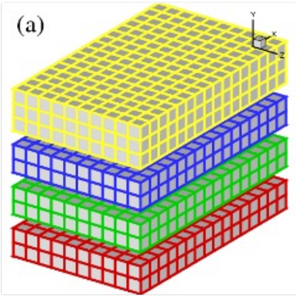
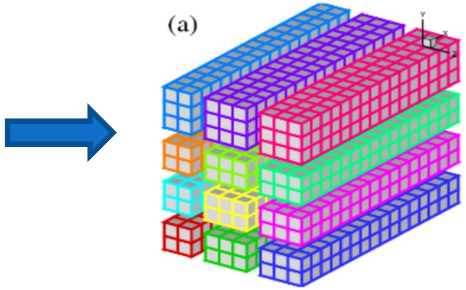
Numerical methods – CHAPSim2

- Domain decomposition - 2decomp&fft library
  - 2-D domain decomposition

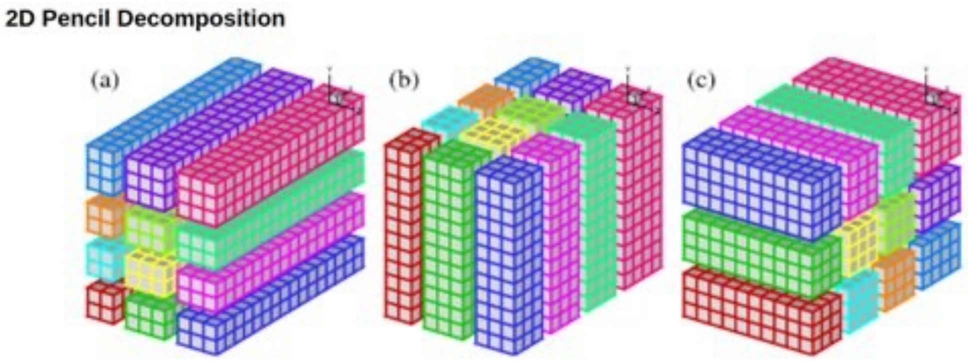


1-D slab
N_core < N in a N*N*Nmesh



2-D pencil
N_core < N*N in a N*N*N mesh

  - Data transport between different pencils



nx=17, ny=13, nz=11, p_row=4, p_col=3

- Application of 2decomp&fft to CHAPSim2 with staggered grids
  - Code

```
!------------------------------------------------------------------------------
! initialize decomp
!------------------------------------------------------------------------------
  call decomp_info_init(dm%np(1), dm%nc(2), dm%nc(3), dm%dpcc) ! for ux, gx
  call decomp_info_init(dm%nc(1), dm%np(2), dm%nc(3), dm%dcpc) ! for uy, gy
  call decomp_info_init(dm%nc(1), dm%nc(2), dm%np(3), dm%dccp) ! for uz, gz
  call decomp_info_init(dm%nc(1), dm%nc(2), dm%nc(3), dm%dccc) ! for p, T, h
  call decomp_info_init(dm%np(1), dm%np(2), dm%nc(3), dm%dppc) ! for intermediate vars
  call decomp_info_init(dm%nc(1), dm%np(2), dm%np(3), dm%dcpp) ! for intermediate vars
  call decomp_info_init(dm%np(1), dm%nc(2), dm%np(3), dm%dpcp) ! for intermediate vars

  call decomp_info_init(dm%np(1), dm%np(2), dm%np(3), dm%dppp) ! this is only used in test.
```

  - Example

```
!------------------------------------------------------------------------------
! calculate div(u_vec)
!------------------------------------------------------------------------------
  div  = ZERO
  accc = ZERO

  call Get_x_1st_derivative_P2C_3D(fl%qx,      accc,         dm, dm%ibcx(:, 1) ) ! accc = d(qx)/d(x)_xccc
  div = div + accc ! = d(qx)/d(x)_ccc

  call Get_y_1st_derivative_P2C_3D(qy_ypencil, accc_ypencil, dm, dm%ibcy(:, 2) ) ! accc_ypencil = d(qy)/(y)_yccc_ypencil
  call transpose_y_to_x (accc_ypencil, accc,         dm%dccc)                      ! accc = d(qy)/d(y)_yccc
  div = div + accc ! = d(qx)/d(x)_ccc + d(qy)/d(y)_ccc

  call Get_z_1st_derivative_P2C_3D(qz_zpencil, accc_zpencil, dm, dm%ibcz(:, 3) ) ! accc_zpencil = d(qz)/(z)_zccc_zpencil
  call transpose_z_to_y (accc_zpencil, accc_ypencil, dm%dccc)          ! accc_ypencil = d(qz)/(z)_zccc_ypencil
  call transpose_y_to_x (accc_ypencil, accc,         dm%dccc)          ! accc = d(qz)/d(z)_zccc
  div = div + accc ! = d(qx)/d(x)_ccc + d(qy)/d(y)_ccc + d(qz)/d(z)_ccc

  call transpose_x_to_y (div,          div_ypencil,  dm%dccc)
  call transpose_y_to_z (div_ypencil,  div_zpencil,  dm%dccc)
```

Numerical methods – CHAPSim2

- Spatial discretisation: compact schemes
  - First order derivatives
    - convection terms, pressure gradient

$$\alpha f^{(1)}_{i-1} + f^{(1)}_{i} + \alpha f^{(1)}_{i+1} = b\frac{f_{i+2} - f_{i-2}}{4h} + a\frac{f_{i+1} - f_{i-1}}{2h}$$

  - Second order derivatives
    - Viscous terms

$$\beta f''_{i-1} + f''_{i} + \beta f''_{i+1} = d\frac{f_{i+2} - 2f_i + f_{i-2}}{4h^2} + c\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}$$

  - Grid interpolation

$$\alpha f_{i'-1} + f_{i'} + \alpha f_{i'+1} = b\frac{f_{i+1} + f_{i-2}}{2} + a\frac{f_i + f_{i-1}}{2}$$

  - Mesh stretching
    - Physical domain <–> computational domain

$$y = h(\eta), \qquad 0 \le \eta \le 1, \qquad 0 \le y \le L_y$$

The first derivative of $f(y)$ is

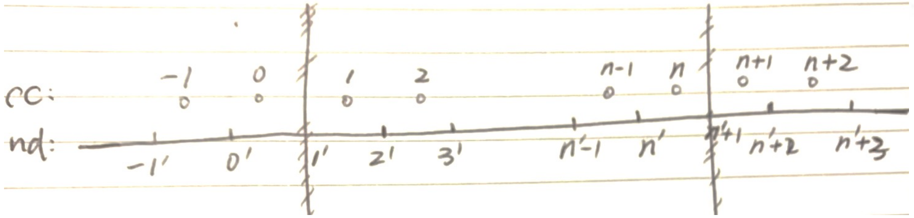
$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial \eta}\cdot\frac{d\eta}{dy} = \frac{1}{dy/d\eta}\frac{\partial f}{\partial \eta} = \frac{1}{h'}\frac{\partial f}{\partial \eta}$$

The second derivative of $f(y)$ is

$$\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right) = \frac{1}{h'^2}\frac{\partial^2 f}{\partial \eta^2} - \frac{h''}{h'^3}\frac{\partial f}{\partial \eta}$$

- Tridiagonal matrix algorithm
  - All data in the same MPI domain
  - Boundary treatment

$$\begin{bmatrix} 1 & \alpha & & & & \alpha \\ \alpha & 1 & \alpha & & & \\ & \alpha & 1 & \alpha & & \\ & & \ddots & \ddots & \ddots & \\ & & & \alpha & 1 & \alpha \\ \alpha & & & & \alpha & 1 \end{bmatrix} \begin{bmatrix} f_1^{(1)} \\ f_2^{(1)} \\ f_3^{(1)} \\ \vdots \\ f_{n-1}^{(1)} \\ f_n^{(1)} \end{bmatrix} = \begin{bmatrix} \frac{b}{4h}(f_3 - f_{n-1}) + \frac{a}{2h}(f_2 - f_n) \\ \frac{b}{4h}(f_4 - f_n) + \frac{a}{2h}(f_3 - f_1) \\ \frac{b}{4h}(f_5 - f_1) + \frac{a}{2h}(f_4 - f_2) \\ \vdots \\ \frac{b}{4h}(f_1 - f_{n-3}) + \frac{a}{2h}(f_n - f_{n-2}) \\ \frac{b}{4h}(f_2 - f_{n-2}) + \frac{a}{2h}(f_1 - f_{n-1}) \end{bmatrix}$$



$$f^{(1)}_{1'} + \alpha f^{(1)}_{2'} = \frac{1}{h}\left(af_{1'} + bf_{2'} + cf_{3'}\right)$$

$$f^{(1)}_{1} + \alpha f^{(1)}_{2} = \frac{1}{h}\left(af_{1'} + bf_{1} + cf_{2} + df_{3}\right)$$

Numerical methods – CHAPSim2

- Compact schemes – code
  - Input:
    - Primary variables at cell centre (C) or grid point (P)
  - Output:
    - First/second derivatives at cell centre (C) or grid points (P)
  - Example:
    - use operations

```
!----------------------------------------------------------------------------------------------
! X-pencil : X-mom convection term (x-c1/3): d(gx * qx)/dx at (i', j, k)
!----------------------------------------------------------------------------------------------

    if ( dm%ithermo == 0) then
      do m = 1, 2
        fbc(m) = dm%fbcx(m, 1) * dm%fbcx(m, 1)
      end do
      call Get_x_1st_derivative_P2P_3D(-fl%qx * fl%qx, apcc, dm, dm%ibcx(:,1), fbc(:) )
    end if
    if ( dm%ithermo == 1) then
      do m = 1, 2
        fbc(m) = dm%fbcx(m, 1) * dm%fbcx(m, 1) * dm%fbc_dend(m, 1)
      end do
      call Get_x_1st_derivative_P2P_3D(-fl%gx * fl%qx, apcc, dm, dm%ibcx(:,1), fbc(:) )
    end if
    fl%mx_rhs = fl%mx_rhs + apcc
```

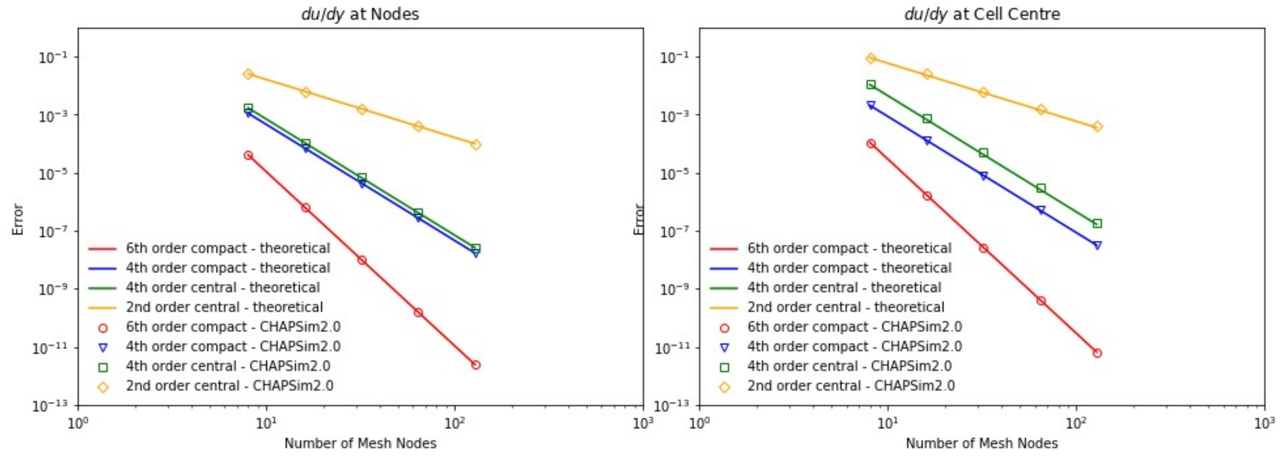
```
public   :: Get_x_midp_C2P_3D
public   :: Get_y_midp_C2P_3D
public   :: Get_z_midp_C2P_3D
public   :: Get_x_midp_P2C_3D
public   :: Get_y_midp_P2C_3D
public   :: Get_z_midp_P2C_3D
```

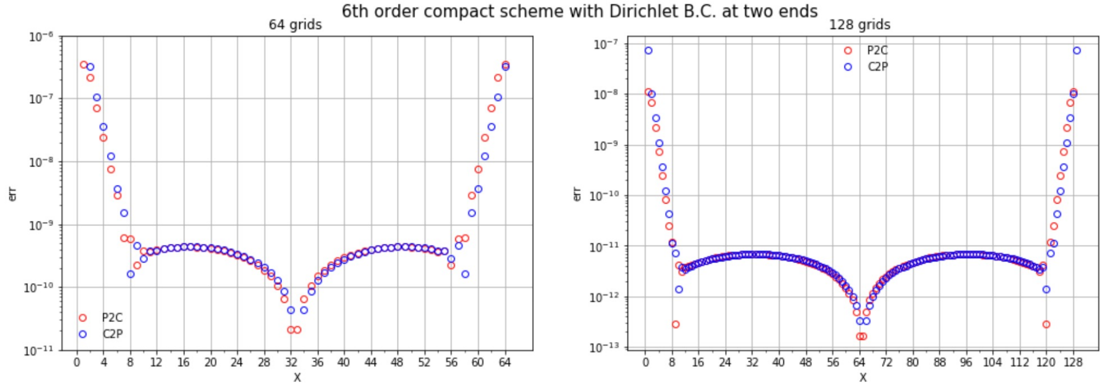
```
public   :: Get_x_1st_derivative_P2P_3D
public   :: Get_y_1st_derivative_P2P_3D
public   :: Get_z_1st_derivative_P2P_3D

public   :: Get_x_1st_derivative_C2P_3D
public   :: Get_y_1st_derivative_C2P_3D
public   :: Get_z_1st_derivative_C2P_3D

public   :: Get_x_1st_derivative_C2C_3D
public   :: Get_y_1st_derivative_C2C_3D
public   :: Get_z_1st_derivative_C2C_3D

public   :: Get_x_1st_derivative_P2C_3D
public   :: Get_y_1st_derivative_P2C_3D
public   :: Get_z_1st_derivative_P2C_3D
```

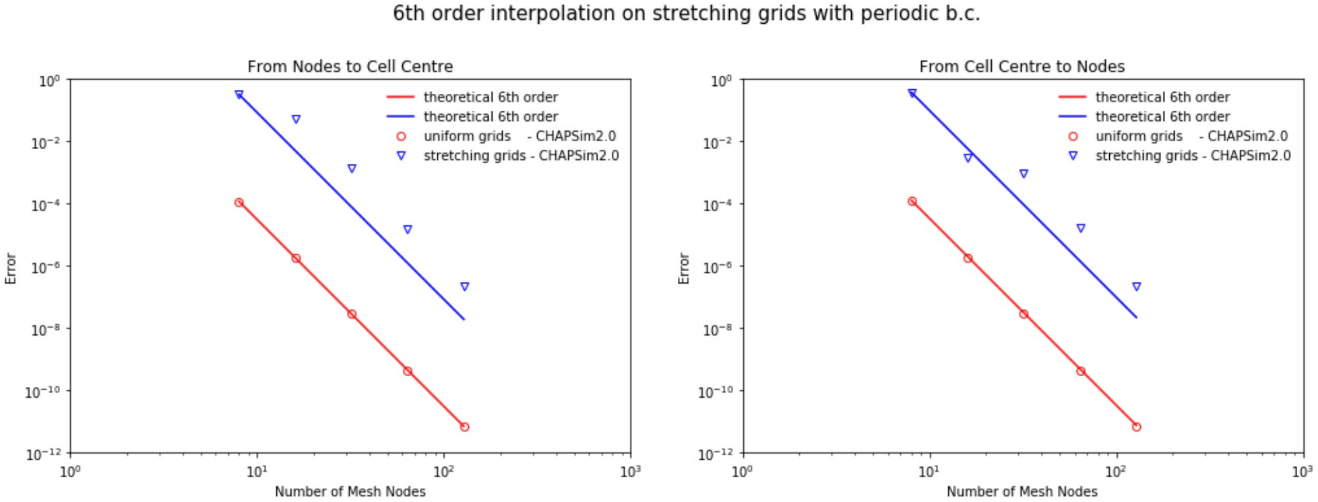
```
public   :: Get_x_2nd_derivative_C2C_3D
public   :: Get_y_2nd_derivative_C2C_3D
public   :: Get_z_2nd_derivative_C2C_3D

public   :: Get_x_2nd_derivative_P2P_3D
public   :: Get_y_2nd_derivative_P2P_3D
public   :: Get_z_2nd_derivative_P2P_3D
```

Numerical methods – CHAPSim2

- Compact schemes – validation







- Up to 6^{th} order accuracy is achieved.
- Stretching grids slightly degrades the accuracy
- Dirichlet boundary condition degrade the accuracy to 3^{rd} order, influencing up to 8 nodes from the boundary.

Numerical methods – CHAPSim2

- Solving Poisson equation

The pressure Poisson equation is

$$\left(\frac{\delta^2}{\delta x_1^2}+\frac{\delta^2}{\delta x_2^2}+\frac{\delta^2}{\delta x_3^2}\right)(\phi)=\frac{\delta u_i}{\delta x_i}\frac{1}{\alpha_1\Delta t}$$

Expressing the terms in the LHS with its FFT,

$$\widehat{f'}_l=\iota\tilde{\kappa}_x\hat{f}_l$$

$$\boxed{\tilde{\kappa}_x=\frac{a\sin(\kappa_x\Delta x)+b/2\sin(2\kappa_x\Delta x)}{\Delta x\cdot(1+2\alpha\cos(\kappa_x\Delta x))}}$$

Extending to the second derivative,

$$\widehat{f''}_l=\iota\tilde{\kappa}_x\widehat{f'}_l=\iota\tilde{\kappa}_x\iota\tilde{\kappa}_x\hat{f}_l=-\tilde{\kappa}_x^2\hat{f}_l$$

Applying 3-D FT to Poisson equation

$$\left(\frac{\delta^2}{\delta x_1^2}+\frac{\delta^2}{\delta x_2^2}+\frac{\delta^2}{\delta x_3^2}\right)(\phi)=\frac{\delta u_i}{\delta x_i}\frac{1}{\alpha_1\Delta t}$$

$$\Leftrightarrow$$

$$\phi''_x+\phi''_y+\phi''_z=D$$

$$\boxed{-(\tilde{\kappa}_x^2+\tilde{\kappa}_y^2+\tilde{\kappa}_z^2)\hat{\phi}_{lmn}=\hat{D}_{lmn}}$$

- Physical domains with stretching grids and non-periodic bc:
  - Grid stretching method with only three Fourier modes in spectral space is applied for a low computational cost (reference: Laizet & Lamballais 2009)

Following the technique introduced by [4], a metric, expressed with only three Fourier modes in spectral space, is proposed here with

$$\frac{1}{h'}=\frac{1}{L_y}\left\{\frac{\alpha}{\pi}+\frac{1}{\pi\beta}\sin^2(\pi(\gamma s+\delta))\right\}=\frac{1}{L_y}\left\{\frac{\alpha}{\pi}+\frac{1}{2\pi\beta}\left[1-\frac{e^{\iota 2\pi(\gamma s+\delta)}+e^{-\iota 2\pi(\gamma s+\delta)}}{2}\right]\right\} \tag{53}$$

so that the mapping (45) can be written as

$$h=\frac{L_y\sqrt{\beta}}{\gamma\sqrt{\alpha}\sqrt{\alpha\beta+1}}\left\{\tan^{-1}\left[\frac{\sqrt{\alpha\beta+1}\tan(\pi(\gamma s+\delta))}{\sqrt{\alpha}\sqrt{\beta}}\right]+\pi\left[H\left(s-\frac{1-2\delta}{2\gamma}\right)+H\left(s-\frac{3-2\delta}{2\gamma}\right)\right]-\tan^{-1}\left[\frac{\sqrt{\alpha\beta+1}\tan(\pi\delta)}{\sqrt{\alpha}\sqrt{\beta}}\right]\right\} \tag{54}$$

$$\left.\widehat{\frac{\partial f}{\partial y}}\right|_m=\sum_{p=-n_y/2}^{n_y/2-1}\hat{a}_p\left.\widehat{\frac{\partial f}{\partial s}}\right|_{m-p}\quad\text{for}\quad -n_y/2\leqslant m\leqslant n_y/2-1$$

the convolution product involves N^2 multiplication.

$$\hat{a}_0=\frac{1}{L_y}\left(\frac{\alpha}{\pi}+\frac{1}{2\pi\beta}\right),\qquad \hat{a}_1=\hat{a}_{-1}=-\frac{1}{L_y}\left(\frac{\cos 2\pi\delta}{4\pi\beta}\right)$$

Numerical methods – CHAPSim2

- Parallel I/O
  - decomp_2d_write/read_one (ipencil, var, filename, opt_decomp)
  - decomp_2d_write/read_var (fh, disp, ipencil, var, opt_decomp)
  - decomp_2d_write/read_scalar (fh, disp, n, var)
  - decomp_2d_write/read_plane (ipencil, var, iplane, n, filename, opt_decomp)
  - decomp_2d_write/read_every (ipencil, var, iskip, jskip, kskip, filename, from1)
- Data visualisation
  - on-the-fly: vtk of each rank
  - post-vtk: an independent postprocessing code for data generated by CHAPSim2
  - Format: vtk
  - Viewer: paraview

Development Plan for the next 12 months

- Code Performance Optimization in ARCHER2
- Port the boundary layer turbulent flow treatment from CHAPSim1 to CHAPSim2
  - Main contributor: Matthew Falcone, Wei Wang
- Port the conjugate heat transfer treatment from CHAPSim1 to CHAPSim2
  - Main contributor: Wei Wang, Jundi He
- Implement the immersed boundary method to CHAPSim2
  - Main contributor: Kenneth Chinembiri, Wei Wang

Groups with Interest in the code

- David Emerson's group, STFC Daresbury Laboratory, UK
- Shiusheng He's group, University of Sheffield, UK
- Mehdi Seddighi's group, Liverpool John Moores University, UK
- Ran Tian's group, Beijing institute of technology, China
- Peixue Jiang's group, Tsinghua University, China
- Walter Ambrosini's group, University of Pisa, Italy
- **Users support and forum**
  - https://join.slack.com/t/chapsim/shared_invite/zt-107i8w8hv-zX8sUSvAczkpxZ21I_HqPQ
  - Discuss applications, report bugs, general questions …

How to get CHAPSim

- CHAPSim Website:
  - https://ccpnth.ac.uk/?page_id=25999
- CHAPSim1
  - https://github.com/CHAPSim/CHAPSim1.0
  - git clone git@github.com:CHAPSim/CHAPSim1.0.git
- CHAPSim2
  - https://github.com/CHAPSim/CHAPSim2
  - git clone git@github.com:CHAPSim/CHAPSim2.git
- Code Structure

CHAPSim updated ignore file	ccf98a1 3 minutes ago	150 commits
example	Added visulisation	2 days ago
lib	updated examples	3 days ago
post_vtk	cleanup	3 days ago
src	added comments	6 minutes ago
.DS_Store	added comments	6 minutes ago
.gitignore	updated ignore file	3 minutes ago
LICENSE	cleanup	3 days ago
Makefile	Added visulisation	2 days ago
README.md	Update README.md	2 hours ago

- Prepare before \`make\`
  - mkdir bin obj mod
- Makefile
  - Production mode
    - make all
  - Testing/debugging mode
    - make cfg=gnu
    - make cfg=intel
    - make cfg=cray
- Demo

How to configure CHAPSim2 input file

- ../../../../../../../Users/wei.wang/Work/11_CHAPSim/CHAPSim/CHAPSim2/example/CHANNEL/input_chapsim_channel.ini

How to run CHAPSim2 on Archer2

- Demo

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Thank you

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CoSeC Computational Science Centre for Research Communities

CCP NTH

UK FLUIDS NETWORK

Questions?

CHAPSim2 - Performance

CHAPSim – Optimisation