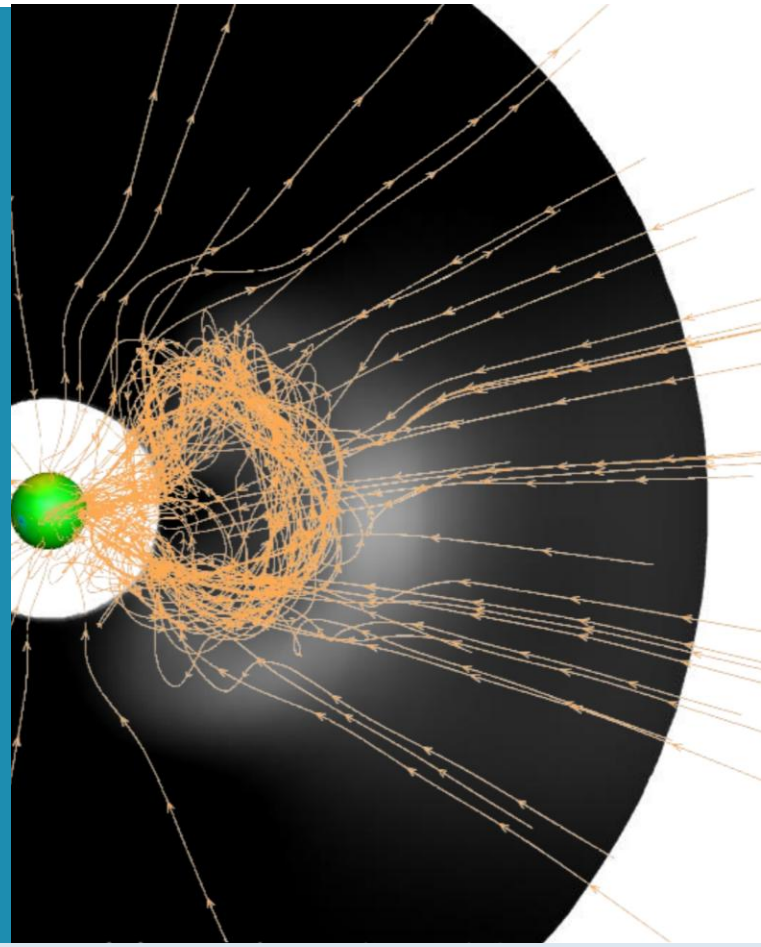
KU LEUVEN

HERCORE: Highly Efficient and quasi-Realistic CORonal and coronal mass Ejection modeling



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KU Leuven, 02/10/2025

Installation of COCONUT

From master version shared on GitHub

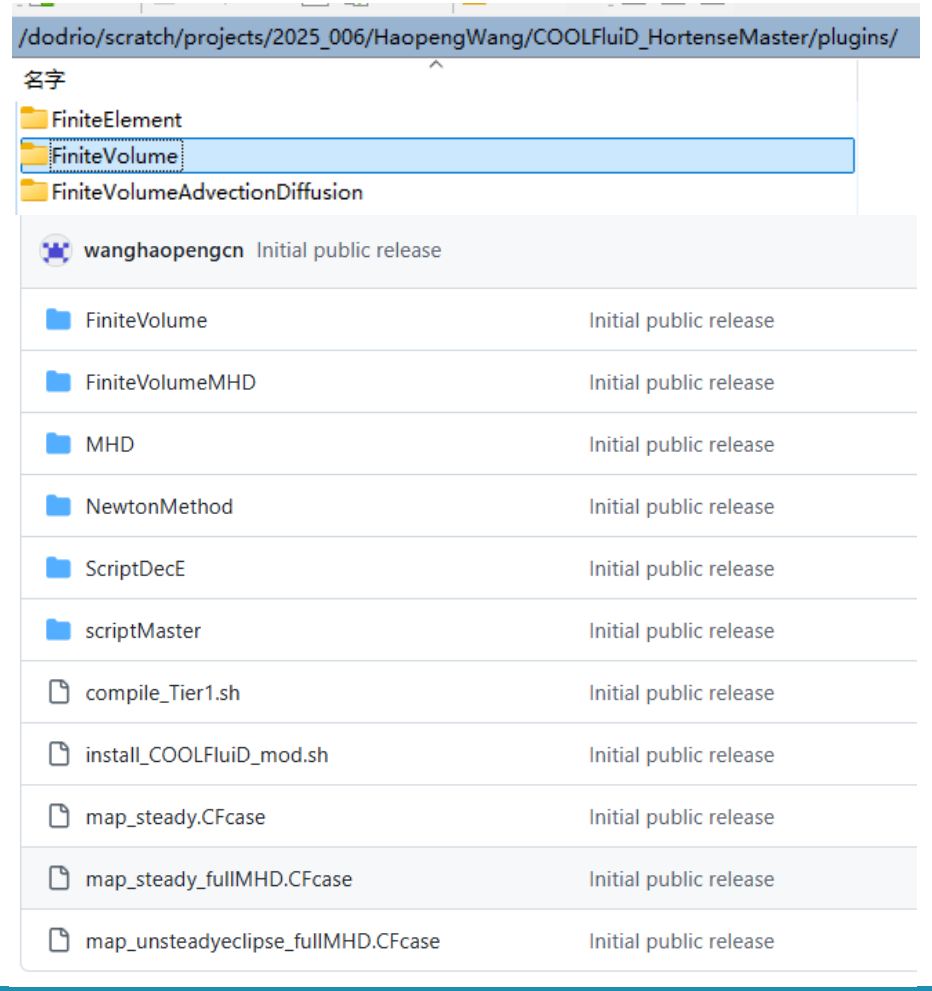
- All source code files, job submission scripts, and installation and recompilation scripts are shared via GitHub or OneDrive. You can directly upload the files from the ***first four folders*** into the corresponding directories in the ***plugins*** folder of the Master version of COCONUT you just installed.
- Before recompile, you need to open the already replaced files, add a space in any blank area, and then save them. This will ensure the replaced files are recognized as modified and will be recompiled.
- ***ScriptDecE*** and ***scriptMaster*** contain job submission scripts corresponds to COCONUT adopting decomposed and full energy equations.

- **Shared via GitHub:** https://github.com/wanghaopengcn/Start-from-COCONUT-HW

wanghaopengcn/Start-from-COCONUT-HW: This repository shares several modifications made to the coronal model COCONUT.

- **Shared via OneDrive:**

Start_from_Master_Version_COCONUT

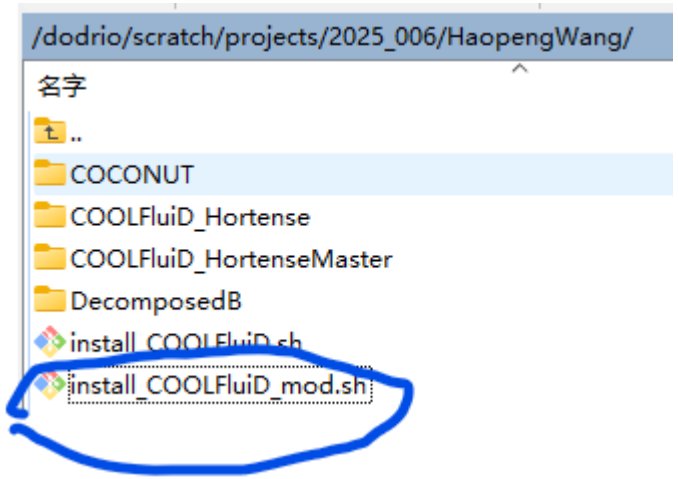


Installation of COCONUT

From master version shared on GitHub

Installation of master version COCONUT on Tier1

1. Modify the path definition of “TOP_DIR” and “COOLFLUID_TOP_DIR” in the script “install_COOLFluiD_mod.sh” according to your case.
2. Via permission of visiting the installation script and execute installation:
   chmod a+x ./install_COOLFluiD_mod.sh
   ./install_COOLFluiD_mod.sh DEBUG NOCUDA –download=2



install_COOLFluiD_mod.sh

```
29  module load CMake/3.26.3-GCCcore-12.3.0
30  module load PETSc/3.20.3-foss-2023a
31
32  export TOP_DIR="${VSC_SCRATCH_PROJECTS_BASE}/2025_006/HaopengWang/"
33  export COOLFLUID_TOP_DIR="${TOP_DIR}/COOLFluiD_HortenseMaster/"
```

vsc35794@login58:/dodrio/scratch/projects/2025_006/HaopengWang

```
   81 |    throw (Common::NoSuchValueException)
      |    ^~~~~
cclplus: note: unrecognized command-line option '-Wno-dev' may have been intended to silence earlier diagnostics
[  7%] Building CXX object src/Framework/CMakeFiles/Framework.dir/DetermineCFL.cxx.o
```

Installation of COCONUT

From master version shared on GitHub

Revision of the master version shared on GitHub

Venktn3DStrict.hh

- Add std::vector<CFuint> _NoLimiterID; (Variables which don't implement limiter)

Venktn3DStrict.cxx

- Add the following snippet to abandon limiter for the selected variables.

```
if (_NoLimiterID.size() > 0){
for (CFuint iVar = 0; iVar < _NoLimiterID.size(); ++iVar){
limiterValue[_NoLimiterID[iVar]] = 1.0;
}
}
```

Venktn3DStrict.hh*

```
protected:
  CFreal _strictCoeff;

  bool _psiMinEqual1;

  /// corresponding to variables which do
  std::vector<CFuint> _NoLimiterID;
```

Venktn3DStrict.cxx

```
    limiterValue[iVar] = psimin;

    const CFreal maxAllowableLimiterFunctionValue = 1.094;
    if (limiterValue[iVar] > maxAllowableLimiterFunctionValue) {
      CFout << "wrong limiterValue = " << limiterValue[iVar] << "\n";
    }
  }
  //>> Mark 2025.07.30 by Hp to cancel limiter for several reconstructed variables
  if (_NoLimiterID.size() > 0){
      for (CFuint iVar = 0; iVar < _NoLimiterID.size(); ++iVar){
          limiterValue[_NoLimiterID[iVar]] = 1.0;
      }
  }
  //<< Mark 2025.07.30 by Hp to cancel limiter for several reconstructed variables
}
```

Venktn3DStrict.cxx MHD3DConsToPrimEInRef.hh

```
  options.addConfigOption< CFreal >
    ("strictCoeff","Fix for smooth flow region.");
  options.addConfigOption< bool >
    ("psiMinEqual1","impose psimin = 1 for certain v
  options.addConfigOption< vector<CFuint> >
      ("NoLimiterID", "Used to cancel limiter.");
}
```

Venktn3DStrict.hh Venktn3DStrict.cxx map_ur

```
Venktn3DStrict::Venktn3DStrict(const std::str
  Venktn2D(name),
  socket_uZ("uZ")
{
  addConfigOptionsTo(this);

  _strictCoeff = 1.0;
  setParameter("strictCoeff",&_strictCoeff);

  _psiMinEqual1 = false;
  setParameter("psiMinEqual1",&_psiMinEqual1)

  _NoLimiterID = vector<CFuint>();
  setParameter("NoLimiterID", &_NoLimiterID);
}
```

Installation of COCONUT

From master version shared on GitHub

Revision of the master version shared on GitHub

StdUpdateSolPP.hh

- Add CFreal _pBC; & CFreal _rhoBC; (It corresponds to boundary density and pressure)

StdUpdateSolPP.cxx

- Add the following snippet to define boundary pressure and density via .Cfcase file.

```
options.addConfigOption< CFreal >("pressureBoundaryValue", "the boundary-pressure value for the pressure.");
options.addConfigOption< CFreal >("densityBoundaryValue", "the boundary-density value for the pressure.");
```

- Comment out CFreal _rhoBC=2.0; & CFreal _pBC = 0.25801090625;

CMakeLists.txt

Move “StdUpdateSolPP.hh” & “StdUpdateSolPP.cxx” from “LIST (APPEND NewtonMethodMHD_files” to “LIST (APPEND NewtonMethod_files”

StdUpdateSolPP.hh | StdUpdateSolPP.cxx

```
//CFreal _rhoBC=2.0;
//CFreal _pBC = 0.25801090625;
CFreal Bmagmax=1.0;
```

StdUpdateSolPP.hh* | StdUpdate

```
bool m_validate;

/// boundary pressure val
CFreal _pBC;
/// boundary plasma densi
CFreal _rhoBC;

}; // class StdUpdateSolPP
```

StdUpdateSolPP.hh | StdUpdateSolPP.cxx*

```
void StdUpdateSolPP::defineConfigOptions(Config::OptionList& options)
{
  options.addConfigOption<vector<CFreal>,Config::DynamicOption<> >("Relaxation","Relaxation factor");
  options.addConfigOption< bool >("Validate","Check that each update creates variables with physical meaning");
  options.addConfigOption< CFreal >("pressureBoundaryValue", "the boundary-pressure value for the pressure.");
  options.addConfigOption< CFreal >("densityBoundaryValue", "the boundary-density value for the pressure.");
}
```

StdUpdateSolPP.hh | StdUpdateSolPP.cxx*

```
StdUpdateSolPP::StdUpdateSolPP(const std::string& name)
  NewtonIteratorCom(name),
  socket_states("states"),
  socket_rhs("rhs"),
  socket_updateCoeff("updateCoeff"),
  socket_invalidStates("invalidStates")
{
  addConfigOptionsTo(this);

  m_alpha = vector<CFreal>();
  setParameter("Relaxation",&m_alpha);

  m_validate = false;
  setParameter("Validate",&m_validate);

  _pBC = MathTools::MathConsts::CFrealEps();
  setParameter("pressureBoundaryValue", &_pBC);

  _rhoBC = MathTools::MathConsts::CFrealEps();
  setParameter("densityBoundaryValue", &_rhoBC);
}
```

Installation of COCONUT

From master version shared on GitHub

Recompile the master version COCONUT on Tier1

1. Modify the path definition of “TOP_DIR” and “COOLFLUID_TOP_DIR” in the script “compile_Tier1.sh” according to your case.
2. Go to the OPENMPI directory where you upload the recompile script “compile_Tier1.sh” and execute recompile via:

- sh compile_Tier1.sh

compile_Tier1.sh

```
module load CMake/3.26.3-GCCcore-12.3.0
module load PETSc/3.20.3-foss-2023a
export TOP_DIR="/readonly${VSC_SCRATCH_PROJECTS_BASE}/2025_006/HaopengWang/"
export COOLFLUID_TOP_DIR="${TOP_DIR}/COOLFluiD_HortenseMaster"

export BUILD_MODE=optim
export CONF_FILE="COOLFluid_Hortense_nocuda.conf"


export COOLFLUID_BASEBUILD_DIR="${COOLFLUID_TOP_DIR}/OPENMPI"
export COOLFLUID_CONF_FILE="${COOLFLUID_TOP_DIR}/${CONF_FILE}"
export COOLFLUID_INSTALL_DIR="${COOLFLUID_BASEBUILD_DIR}/${BUILD_MODE}/INSTALL"
export ALL_ACTIVE=1

cd $COOLFLUID_TOP_DIR
#./prepare.pl --config-file=${COOLFLUID_CONF_FILE} --build=${BUILD_MODE}

cd ${COOLFLUID_BASEBUILD_DIR}/${BUILD_MODE}
make -j 4
#make install
```

```
[vsc35794@login58 ~]$ cd /dodrio/scratch/projects/2025_006/HaopengWang/COOLFluiD_HortenseMaster/OPENMPI/
[vsc35794@login58 OPENMPI]$ sh compile_Tier1.sh
```

Installation of COCONUT

From master version shared on GitHub

1st step: Polytropic quasi-steady-state simulation on Tier1

Revise the following configuration in map_steady.Cfcase

- Simulator.Paths.ResultsDir = ./results-map-res/30Rs_lvl6/steady/polytropic/ADAPT2008/lmax25
- Simulator.SubSystem.EM.Data.DistanceBased.FileNameTw= ./MapData/ADAPT2008Lmax25/map_adapt_lmax25_20080803140000.dat
- Simulator.SubSystem.Flow.Data.DistanceBased.FileNameTw = ./MapData/ADAPT2008Lmax25/map_adapt_lmax25_20080803140000.dat
- Simulator.SubSystem.Flow.Data.Venktn3DStrict.NoLimiterID = 1 2 3 4 5 6
- Simulator.SubSystem.CFmesh1.FileName = corona_NoLim_PPDecEBC1_20080803ADAPT.Cfmesh
- Simulator.SubSystem.Tecplot1.FileName = corona_NoLim_PPDecEBC1_20080803ADAPT.plt
- Simulator.SubSystem.FlowIterator.StdUpdateSolPP.pressureBoundaryValue =0.108 #0.25801090625
  Simulator.SubSystem.FlowIterator.StdUpdateSolPP.densityBoundaryValue =1.0 #2.0
- The following boundary conditions should be revised according to your cases.
  Simulator.SubSystem.Flow.Jet1.rhoBC = 1.0 #1.0
  Simulator.SubSystem.Flow.Jet1.pBC = 0.108 #0.00284615174 #0.08592156224 #0.108
  Simulator.SubSystem.Flow.InField.Def = \

Create a symbolic link to the path of the working folder

- ln -sf /dodrio/scratch/projects/2025_006/CompleteCopyTest/COOLFluiD_Hortense/OPENMPI/optim/apps/Solver/coolfluid-solver* ./

Submit a job

- qsub run_Quasi_steady_Tier1.pbs

Installation of COCONUT

From master version shared on GitHub

2nd step: Restart full MHD quasi-steady-state simulation from the polytropic quasi-steady-state simulation results on Tier1

Revise the following configuration in map_steady_fullMHD.Cfcase

- Simulator.Paths.ResultsDir = ./results-map-res/30Rs_lvl6/steady/fullMHD/ADAPT2008/lmax25
- Simulator.SubSystem.CFmeshFileReader0.Data.FileName = ./results-map-res/30Rs_lvl6/steady/polytropic/ADAPT2008/lmax25/corona_NoLim_PPDecEBC1_20080803ADAPT.Cfmesh
- Simulator.SubSystem.CFmeshFileReader1.Data.FileName = ./results-map-res/30Rs_lvl6/steady/polytropic/ADAPT2008/lmax25/corona_NoLim_PPDecEBC1_20080803ADAPT.Cfmesh
- Simulator.SubSystem.Flow.Restart = true
- The other revisions are like those modifications in map_steady.Cfcase

Submit a job

- qsub run_Quasi_steadyfullMHD_Tier1.pbs

```
cd /dodrio/scratch/projects/2025_006/HaopengWang/COCONUT/
##module swap cluster/dodrio/cpu_rome_512
module load CMake/3.26.3-GCCcore-12.3.0
module load PETSc/3.20.3-foss-2023a
module load vsc-mympirun
mympirun --universe 360 ./coolfluid-solver --scase /dodrio/
```

Installation of COCONUT

From master version shared on GitHub

3rd step: Restart time-evolving coronal simulation from full MHD quasi-steady-state simulation results on Tier1

Pay attention to the following modification in *map_steady_fullMHD.Cfcase*

- Simulator.SubSystem.FlowSubSystemStatus.TimeStep = 0.207297 # Corresponds to 5 minutes
- Simulator.SubSystem.InitialTime = 0.0 # In code hour unite, the restart physical time *3600.0/1447.2
- Simulator.SubSystem.MaxTime.maxTime = 1641.79 # End of the physical time *3600.0/1447.2
- Simulator.SubSystem.Flow.Data.DistanceBased.FileNameTwADF = ./MapData/zqsCR2296Lmax25/map_gong_lmax25_2025 0400.dat 663 1 2025 32919 32918 # Require to be revised according to your cases.
- Simulator.SubSystem.Flow.Data.Venktn3DStrict.NoLimiterID = 1 2 3 4 5 6 # variables which don't implement limiter
- Simulator.SubSystem.Flow.Data.HLL.AddLax = true # true for decomposed energy equation
- The other revisions are like those modifications in map_steady.Cfcase
- Comment out *Simulator.SubSystem.Flow.Jet1.VarIDs = 0* will trun the time-evolving regime to quasi-steady-state regime.
- Pay attention to comments starting with # Decomposed energy
- Also refer to the papers and manuals contained in the **eDocuments** folder for further reference.

Submit a job

- qsub run_TimeevolvingfullMHD_Tier1.pbs

Installation of COCONUT

From master version shared on GitHub

Calculate source terms as Haopeng Wang did and considering decomposed energy equation.

MHDConsACAHWSourceTerm.cxx

- Add the following snippet for decomposed energy equation

.Cfcase

- Switching to "Simulator.SubSystem.Flow.Data.SourceTerm = MHDConsACAHWST" to calculate source terms as Haopeng Wang did.
- Adding "Simulator.SubSystem.Flow.Data.MHDConsACAHWST.deCompEorNot = 0" means doesn't calculate the source term caused by decomposed energy equation.

onsACAHWSourceTerm.hh | MHDConsACAHWSourceTerm.cxx* | map_steady.CFcase

```
options.addConfigOption< CFint >("RadiativeLossTerm","Switch on optically thin approximation for radiation loss
options.addConfigOption< CFint >("deCompEorNot", "Calculate source term caused by decomposed energy equation.")
```

HDConsACAHWSourceTerm.hh | MHDConsACAHWSourceTerm.cxx

```
setParameter("RadiativeLossTerm",&_RadiativeLossTerm);
_deCompE = 0;
setParameter("deCompEorNot", &_deCompE);
```

MHDConsACAHWSourceTerm.hh

```
CFint _wave_pressure;
CFint _deCompE
```

onsACAHWSourceTerm.hh | MHDConsACAHWSourceTerm.cxx | map_steady.CFcase

```
}

//>> energy Source terms caused by decomposed energy equation
//CFuint deCompE = 1;
CFreal Q_deCompE = 0.0;
//if (deCompE == 1 && r_dimless>1.05){
if (_deCompE == 1){
    const CFuint BXID = 4;
    const CFuint BYID = 5;
    const CFuint BZID = 6;
    const CFuint gradBXID = elementID*nbEqs + BXID;
    const CFuint gradBYID = elementID*nbEqs + BYID;
    const CFuint gradBZID = elementID*nbEqs + BZID;
    _gradBx[XX] = this->m_ux[gradBXID];
    _gradBx[YY] = this->m_uy[gradBXID];
    _gradBx[ZZ] = this->m_uz[gradBXID];
    _gradBy[XX] = this->m_ux[gradBYID];
    _gradBy[YY] = this->m_uy[gradBYID];
    _gradBy[ZZ] = this->m_uz[gradBYID];
    _gradBz[XX] = this->m_ux[gradBZID];
    _gradBz[YY] = this->m_uy[gradBZID];
    _gradBz[ZZ] = this->m_uz[gradBZID];
    std::vector<CFreal> BdotLamdaB(3, 0.0);
    std::vector<CFreal> VdotLamdaB(3, 0.0);
    VdotLamdaB[0] = Vx*_gradBx[XX] + Vy*_gradBx[YY] + Vz*_gradBx[ZZ];
    VdotLamdaB[1] = Vx*_gradBy[XX] + Vy*_gradBy[YY] + Vz*_gradBy[ZZ];
    VdotLamdaB[2] = Vx*_gradBz[XX] + Vy*_gradBz[YY] + Vz*_gradBz[ZZ];
    BdotLamdaB[0] = (Bx*_gradBx[XX] + By*_gradBx[YY] + Bz*_gradBx[ZZ]) / B0;
    BdotLamdaB[1] = (Bx*_gradBy[XX] + By*_gradBy[YY] + Bz*_gradBy[ZZ]) / B0;
    BdotLamdaB[2] = (Bx*_gradBz[XX] + By*_gradBz[YY] + Bz*_gradBz[ZZ]) / B0;
    Q_deCompE = Vx*BdotLamdaB[0] + Vy*BdotLamdaB[1] + Vz*BdotLamdaB[2] -
        (Bx*VdotLamdaB[0] + By*VdotLamdaB[1] + Bz*VdotLamdaB[2]) / B0;
    source[7] += Q_deCompE*volumes[elementID];
}
//<< energy Source terms caused by decomposed energy equation
```

Installation of COCONUT

From master version shared on GitHub

Considering extra dissipation term for decomposed energy equation.

HLLFlux.cxx & HLLFlux.hh

- Add the following snippet to add extra diffusion term to HLL solver for decomposed energy equation
- Adding "Simulator.SubSystem.Flow.Data.HLL.AddLax = false" to .Cfcase means doesn't consider the extra dissipation term.
- Always keep "Simulator.SubSystem.Flow.Data.HLL.UseAlpha = true".

HLLFlux.hh | HLLFlux.cxx | map_steady

```
setParameter("UseAlpha", &_useAlpha
_addLax = false;
setParameter("AddLax", &_addLax);
}
```

HLLFlux.hh | HLLFlux.cxx

```
/// use alpha coef
bool _useAlpha;

/// Add extra diff
bool _addLax;
```

HLLFlux.cxx | HLLFlux.cxx

```
result = 0.5*(_leftFlux
(amax + amin)/(ama
amax * amin/(amax
}
else {
CFreal alpha=max(abs(am
if (_addLax){
alpha = 1.0;
}
result = 0.5*(_leftFlux
(amax + amin)/(ama
alpha*2.0*amax * a
}
```

Flux.hh | HLLFlux.cxx | map_steady.CFcase

```
void HLLFlux::defineConfigOptions(Config::OptionList& options)
{
options.addConfigOption< bool >("UseAlpha", "Use diffusion reduction coefficient");
options.addConfigOption< bool >("AddLax", "Add extra diffusion term to HLL solver");
}
```

Flux.hh | HLLFlux.cxx | map_steady.CFcase

```
//>> mark 2025.08 by HP
if (_addLax){
GeometricEntity& face = *data.getCurrentFace();
State& left = *face.getState(0);
State& right = *face.getState(1);

CFreal P0 = 0.03851; // N/m**2
CFreal mu0 = 1.2566e-6;
CFreal p_tempL = left[7];
CFreal p_tempR = right[7];
CFreal pthL = p_tempL*P0;
CFreal pthR = p_tempR*P0;
CFreal BxL = left[4];
CFreal ByL = left[5];
CFreal BzL = left[6];
CFreal BxR = right[4];
CFreal ByR = right[5];
CFreal BzR = right[6];
CFreal Bsq2L = BxL*BxL + ByL*ByL + BzL*BzL;
CFreal Bsq2R = BxR*BxR + ByR*ByR + BzR*BzR;
CFreal pmagL = max(Bsq2L / 2. / mu0, 1.e-16);
CFreal pmagR = max(Bsq2R / 2. / mu0, 1.e-16);
CFreal plasmaBetaL = pthL / pmagL;
CFreal plasmaBetaR = pthR / pmagR;
CFreal fac = 1.0;
CFreal Q_BetafactorL = std::tanh(fac / plasmaBetaL / 100.0);
CFreal Q_BetafactorR = std::tanh(fac / plasmaBetaR / 100.0);
CFreal Q_Betafactor = max(Q_BetafactorL, Q_BetafactorR);
result[7] -= 0.125*Q_Betafactor*max(amax, std::abs(amin)) * (rightState[7] - leftState[7]);
}
//<< mark 2025.08 by HP
```

Installation of COCONUT

From master version shared on GitHub

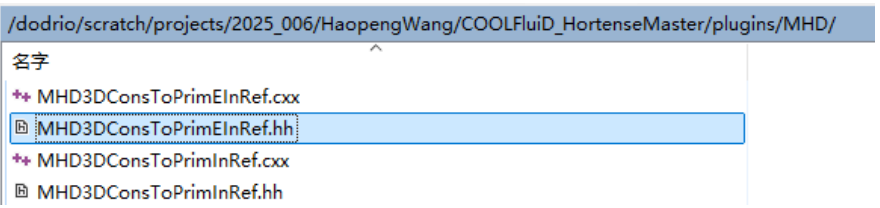
Considering decomposed energy equation.

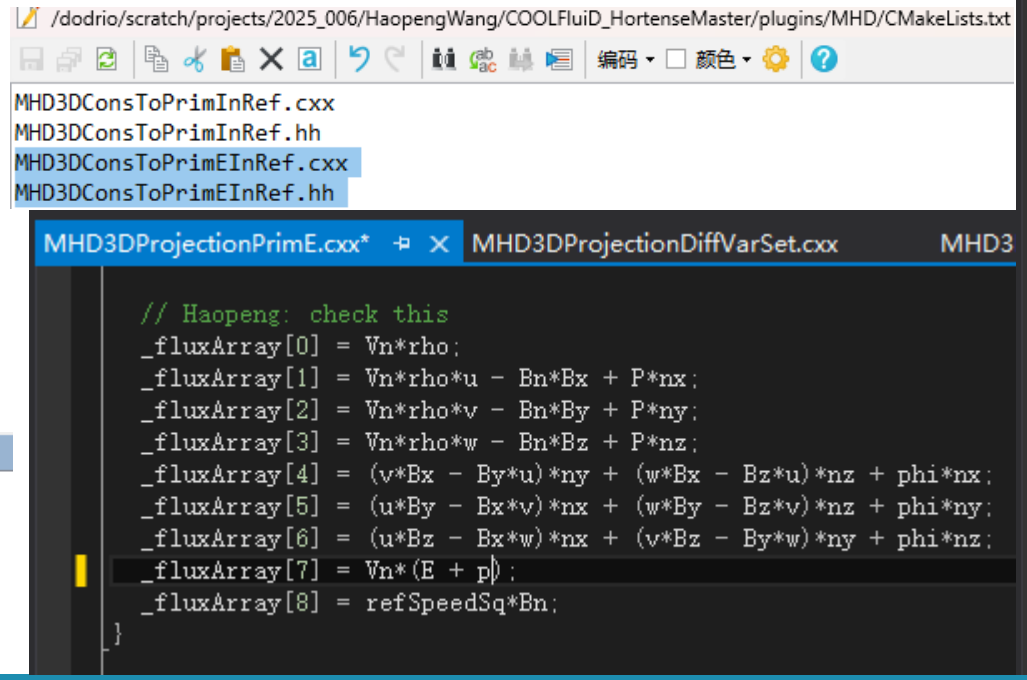
MHD3DProjectionPrimE.cxx

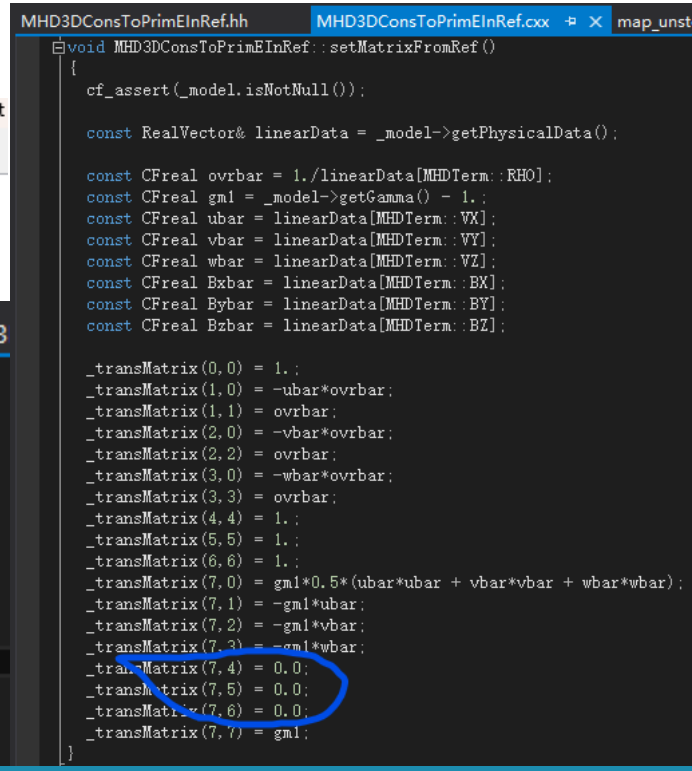
- Correct "_fluxArray[7] = Vn*(E + P);" to "_fluxArray[7] = Vn*(E + p);" for decomposed energy equation

MHD3DConsToPrimEInRef.xx

- Create "MHD3DConsToPrimEInRef.xx" based on "MHD3DConsToPrimInRef.xx", and add the newly created files to CMakeLists.txt







Installation of COCONUT

From master version shared on GitHub

Considering decomposed energy equation.

.Cfcase

- Simulator.SubSystem.Flow.Data.HLL.UseAlpha = true # Use self-adjustable dissipation term for HLL flux solver.
- Simulator.SubSystem.Flow.Data.HLL.AddLax = true # true for decomposed energy equation with addition dissipation term to HLL flux solver
- Simulator.SubSystem.Flow.Data.SourceTerm = MHDConsACAHWST # calculate source terms as Haopeng did.

- Simulator.SubSystem.Tecplot1.Data.outputVar = PrimE # adopt decomposed energy equation
- Simulator.SubSystem.ParaView1.Data.updateVar = PrimE # adopt decomposed energy equation
- Simulator.SubSystem.Flow.Data.UpdateVar = PrimE # adopt decomposed energy equation
- Simulator.SubSystem.Flow.Data.MHDConsACAHWST.deCompEorNot = 1 # 1 for decomposed energy equation with source term caused by decomposed energy equation

- Since the source code is modified for decomposed energy equation, remember to execute recompile before job submission.

Installation of COCONUT

From master version shared on GitHub

Considering full energy equation.

.Cfcase

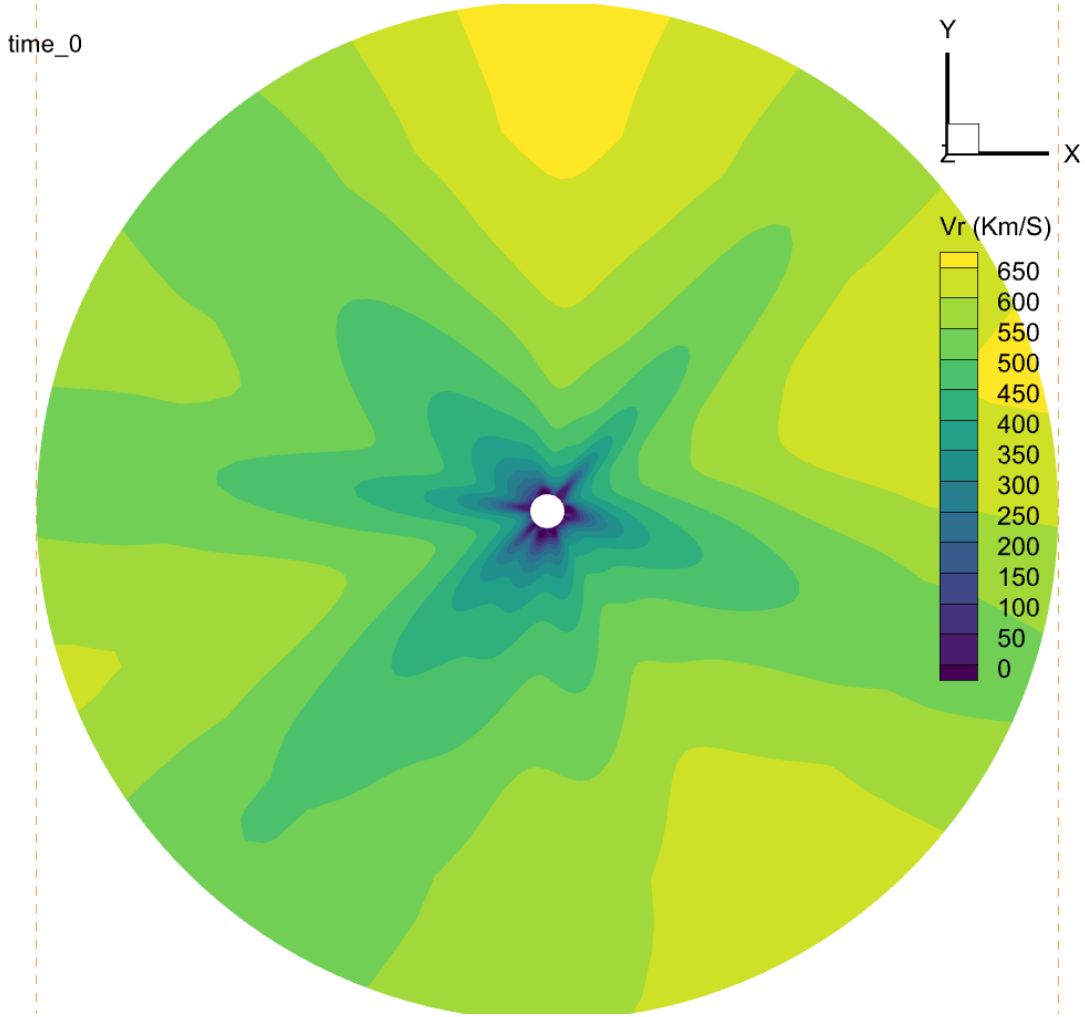
- Simulator.SubSystem.Flow.Data.HLL.UseAlpha = true
- Simulator.SubSystem.Flow.Data.HLL.AddLax = false # false for full energy equation without addition dissipation term to HLL flux solver
- Simulator.SubSystem.Flow.Data.HLL.AddLax = true # true for full energy equation with addition dissipation term to HLL flux solver
- Simulator.SubSystem.Flow.Data.SourceTerm = MHDConsACAHWST # calculate source terms as Haopeng did.

- Simulator.SubSystem.Tecplot1.Data.outputVar = Prim # adopt full energy equation
- Simulator.SubSystem.ParaView1.Data.updateVar = Prim # adopt full energy equation
- Simulator.SubSystem.Flow.Data.UpdateVar = Prim # adopt full energy equation
- Simulator.SubSystem.Flow.Data.MHDConsACAHWST.deCompEorNot = 0 # 0 for full energy equation without source term caused by decomposed energy equation

Installation of COCONUT

From master version shared on GitHub

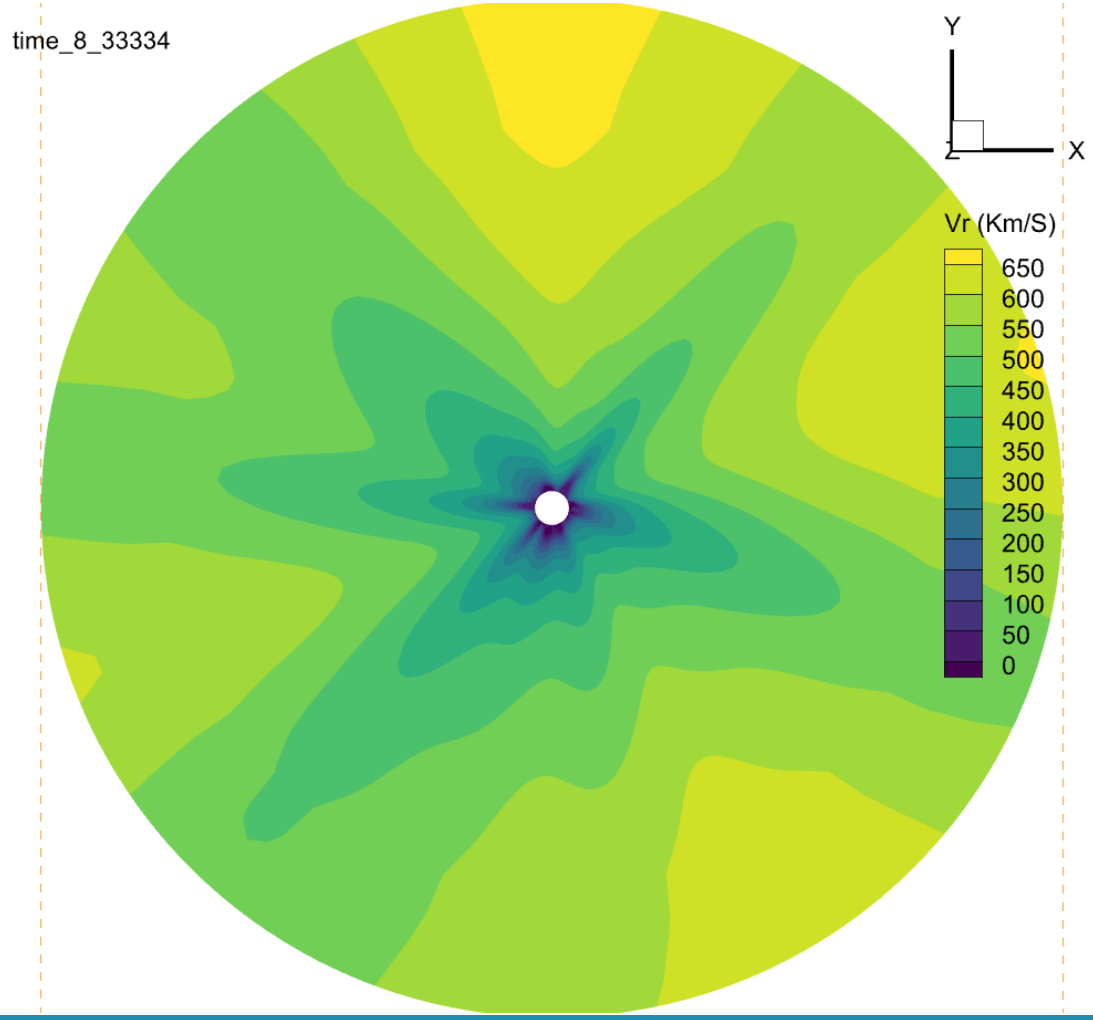
Calculated by full energy equation f or CR2296 (GONGzqs Lmax=25).



Installation of COCONUT

From master version shared on GitHub

Calculated by full energy equation f or CR2296 (GONGzqs Lmax=25).



Call for more collaborations

1. The implicit time-evolving coronal models COCONUT and SIP-IFVM show great promise for **practical space weather forecasting** due to their efficiency and stability. (Providing inner-boundary conditions for inner-heliosphere models, improve efficiency of CME simulations with required accuracy, …)

2. The extended magnetic field decomposition strategy and energy decomposition strategies improve the numerical stability of the MHD coronal and CME models in addressing **time-evolving low-β issues**.

3. We are **extending** the coronal model to 1 AU or **coupling** the coronal model with an inner heliosphere model to conduct some **faster-than-real-time** and more **realistic** CME simulations from the solar surface to 1 AU.

4. We plan to integrate active region models into global coronal model COCONUT.

Looking forward to more good ideas and comments

Thanks

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