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14. ABSTRACT
TURF development has been ongoing at AFRL/RQRS for over two years and has reached a stage where most of the underlying code data-structures and interfaces are at a level of maturity at which it is possible for collaborators to begin writing external modules for the framework. To facilitate bringing these collaborators up to speed in writing modules for TURF, the TURF-IR has the capabilities in place to demonstrate bare-bones kinetic and fluid simulations, including a few example input files to provide convenient starting points for the development of additional physics capabilities. Though the framework has been designed in part to facilitate the creation of modules that replicate the functionality of Coliseum/HPHall, it must be emphasized that the TURF-IR is intended to stimulate academic collaboration and does not provide equivalent real-world capabilities to the Coliseum/HPHall suite. As such, this software by itself cannot be used to design or analyze real systems.

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1. Introduction

TURF development has been ongoing at AFRL/RQRS for over two years and has reached a stage where most of the underlying code data-structures and interfaces are at a level of maturity at which it is possible for collaborators to begin writing external modules for the framework. To facilitate bringing these collaborators up to speed in writing modules for TURF, the TURF-IR has the capabilities in place to demonstrate bare-bones kinetic and fluid simulations, including a few example input files to provide convenient starting points for the development of additional physics capabilities. Though the framework has been designed in part to facilitate the creation of modules that replicate the functionality of Coliseum/HPHall, it must be emphasized that the TURF-IR is intended to stimulate academic collaboration and does not provide equivalent real-world capabilities to the Coliseum/HPHall suite[6, 7, 4]. As such, this software by itself cannot be used to design or analyze real systems.

2. Core Structure

TURF is designed around a basic tree hierarchical object structure. TURF objects are built around this core “General Service Object” or “GObject” that facilitates construction of object trees and allows branches of the tree to be recursively copied across disparate memory spaces such as from the CPU to GPU or across the message passing interface (MPI) without losing their structural integrity. Because TURF objects are all derived from this basic type, in addition to the core functionality required for this recursive data movement, the GObject also facilitates recursive auto-documentation of runtime object structure.

The objects of TURF can be divided between data objects and operation objects. The number of data objects are intentionally restricted to provide a basic common skeleton of data storage on which a broad set of operations can be applied. These basic data objects with minimal independent functionality facilitate code reuse by providing a common basis though which operations interact. They also help simplify parallel communication by minimizing the set of disparate objects that must be transferred. The operation objects define the key application programming interface through which developers are encouraged to interact with the framework. They are intended to represent compact mathematical operations and consist of 3 key components. Every operation includes an “init” function that is passed a map of parameter-key values. It is the operation’s responsibility to parse this map to initialize all
the local information, create data-structures as needed, and query the existing object hierarchy for references to additional required objects needed to function. For some operations such as initial conditions, this initialization is all that is required. For operations that evolve the problem solution, an “apply” function is defined. This function is called as the framework iterates through a sequence of operations to perform a specific function on the data. Whenever possible, this functionality should be further broken down into one or more “core” functions that represent the functionality in a data independent parallel form that is designed to be agnostic to whether the core is applied sequentially on a single process, in parallel through threads or as implemented by OpenMP, or in parallel on an accelerator such as the GPU.

Though additional data-structures may be created and inherited from those already included in the TURF-IR, this practice is discouraged in favor of using existing data-structures to the greatest extent possible so that operations apply in the largest context possible. Both the organizational layout of the data as well as the sequence of operations performed on the data are then constructed at runtime facilitating rapid modular algorithm design. As a result of this highly modular design, library modules of operations can be included or omitted without impacting the functionality of other modules. This “plug-in” model implies that, if a particular release of TURF is missing a module (e.g. a C-R physics module), there are no hooks to indicate that a particular module is missing. In this way, reverse engineering the functionality of a module from the generic interfaces defined by the framework is impossible. For an authorized developer, however, it is critical that the interfaces between their modules and the framework are well-defined. Actually having a copy of the TURF-IR permits them to test the compatibility of their modules within the framework and helps ensure data-structure compatibility and adherence to the module interface for delivered code.

3. Key Data-structures

Creating modules that interface efficiently with TURF requires a detailed understanding of the layout of data in memory (i.e. the data-structures). These underlying data-structures are largely tied to the sort of data being stored (particle/field data) and the sort of mesh on which it is being stored (mesh-free/structured mesh/unstructured mesh) but are all based on a custom multi-dimensional matrix object called gMatrix, a GSOObject encapsulation and extension of the matrix objects used extensively in the AFRL/RQRS’s prior research codes[9, 8, 10, 5, 11]. As a fundamental data object, it is generic templated container class. The mesh classes of SMesh (structured) and UMesh (unstructured) are compound objects of header information and gMatrix objects based on generic mesh classes used also extensively by AFRL/RQRS over the last five years in numerous PhD and Masters theses (refs?).

In addition to mesh objects, the TURF-IR includes examples of basic particle and field data objects with similar header/gMatrix compound structure.

4. Basic Functionality

For this version of the TURF-IR, the computational domain is centered around a constant spaced global Cartesian coordinate system. Though this “LogicalWorld” object is derived from a more general “World” object, the current version of the framework assumes the existence of the global real to logical coordinate system to facilitate domain patching automation while varying resolution. Active regions of the global coordinate system are defined by “LogicalDomain” objects. These are essentially intended to be discrete axis aligned blocks for the sake of domain decomposition. Computation on every domain should be able to run independently of the others except for discrete synchronization points at which time patches between domains are guaranteed to have completed. These synchronization points are the end of computational stages.

Once the world and domains have been created, various “Operations” are applied. These operations can create additional data objects to attach to the domain, set initial and boundary conditions, solve sets of equations, write output, or any number of other manipulations of the data within the framework so long as they may be applied for one domain at a time independently. Communication between domains is restricted to stage boundaries to preserve this independence. The intent of this is two pronged. The first goal is to encourage as much fine grain parallelization as possible. Extremely broad definition of an operation is also intended to avoiding locking the framework to a specific set of applications due to more rigidly defined interfaces and phases of computation. The function of the framework is then an extremely generic statement of, “There exists a set of data on which a sequence of parallel operations may be applied that can be broken down into discrete stages between which communication between the datasets may be performed.” In general, the world typically advances in computational time looping through
the operations, but this functionality is only included to assist in timestep synchronization between domains as this is a commonly required functionality not easily obtainable in a domain independent manner. The form of the time advancement, whether implicit, or explicit, or iteration towards steady state, must be defined as built into the sequence of operations rather than a pre-selected as a trait of the framework.

5. Capabilities

The ultimate capability of TURF-IR is really dictated by how the parts are used together. While TURF-IR is not crippled and is intended to provide reasonable parallel scaling to look at fairly computationally challenging problems. This scaling will be a primary thrust for verification in future infrastructure releases. However, the TURF-IR simply lacks the physics modules to perform real-world simulations. In particular, it does not have any of the sputtering capability nor HPhall interfaces which make the Coliseum suite a tool for realistic spacecraft-thruster interaction modeling. A similar situation exists for the fluid and Vlasov capability in the TURF-IR. They are limited to a low-order and low-dimensionality, respectively, to offer only limited capability for real-world simulation. They do provide enough framework to allow our external collaborators to add different type of high-order solvers at our discretion and to run many fundamental test cases used in evaluating numerical methods.

The visualization capability provided by TURF-IR is the ability to write various VTK output formats for structured/unstructured grids and fields as well as some line plot data output. TURF also includes a compilation flag that allows the framework to be compiled with VisIt (DoE) libSim[15] libraries for near-realtime in-situ visualization. When included, all visualize data-structures such as particle distributions, meshes, and field data are accessible automatically if attached to the GSObject hierarchy from the World. Because this process is automatic, access includes temporary buffered versions of the objects such as ghost and exchange particle distributions which can aid in debugging. Access to data is currently only available between iterations through the entire operation stack, but future versions of TURF may be modified to allow visualization after each operation while in debug mode to facilitate visual debugging. The libSim functionality is still experimental and currently only operational on a single MPI process, though the interface was designed for full parallel scalability.

Table 1 below provides a list of Operations included in the TURF-IR with short descriptions which are used in the accompanying tutorials covering a particle heatbath[13, 14], direct simulation Monte Carlo 1D shock [1], a 1D1V collisionless electrostatic shock [3], and a 3D3V electrostatic collisionless particle in cell test case[12].

6. Extended Capabilities

Beyond the material covered in the tutorial, several additional tutorials are currently being developed. These include a PIC and Fluid versions of the collisionless shock tutorial using the same problem setup[2], ionizing breakdown using MCC collisions with particle merging and splitting, 1D Euler shock tube and 3D Euler shock-bubble fluid test cases, 3D DSMC bow-shock examples for both geometrically prescribed bodies as well as triangulated surface meshes, and a GPU accelerated version of the heatbath tutorial. Many of the Operations required for development of these tutorials are already complete but are not yet ready to be incorporated into the infrastructure release. The intent is to transition many of these Operations into the infrastructure in the next infrastructure release. These operations may nevertheless be available to select developers as part of the thermophysics universal research framework development (TURF-DEV) package on a case-by-case basis. Brief descriptions of the operations are provided in Table 2.

In addition to the TURF-DEV operations nearing incorporation in the infrastructure, another class of TURF-DEV operations are available that are still in experimental phases of development or are potentially too specific research problem dependent to warrant inclusion in the infrastructure. Brief descriptions of these operations are included in Table 3 as reference for some future areas of development.

7. Conclusion

The TURF-IR is an interim release intended to stimulate collaboration by demonstrating code data structures and interfaces in the context of very basic fluid and kinetic simulation capabilities; however, by itself, this software cannot be used to design or analyze real systems.
Table 1. Summary of operations included in TURF-IR.

<table>
<thead>
<tr>
<th>Module</th>
<th>Operation Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DSMC</td>
<td>SPDistDSMCConstantICOp: Initial distribution of particles inside the domain</td>
</tr>
<tr>
<td>DSMC</td>
<td>SPDistDSMCOp: DSMC collision calculation</td>
</tr>
<tr>
<td>DSMC</td>
<td>SPDistDSMCSampleOp: Blend running average of field data</td>
</tr>
<tr>
<td>DSMC</td>
<td>SPDistDSMCSampleOp: Sample particles</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalBCConstantOp: Set value of cell centers in box every iteration</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalBCXtrapOp: Sets a physical boundary to extrapolation</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalFieldAddOp: Adds one field variable to another</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalFieldScalarMulOp: Multiplies field by scalar constant</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalFieldSetOp: Set field values to constant</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalFieldSetOp: Initialize the field parameters</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalFieldVolumetricMulOp: Multiplies or divides field data by cell volumes</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalGradientCellCenterOp: Calculates the gradient of a field vector</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalNodeGradientOp: Calculate node-centered gradient of cell center field</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalNormOp: Calculate $L^p$-norm of field variable</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalPoissonBoltzmannStrip1DOp: Solves for the electric field assuming Boltzmann electrons</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalPoissonStripOp: Red/Black line relaxing Poisson solve</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalResidualOp: Calculate residual of Poisson solve</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistBCSpecOp: Specularly reflecting boundary condition</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistCellIDOp: Find cell ID associated with particle location</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistCombineOp: Unifies the particles from different distributions</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistConstantBCOp: Add Particles in box with uniform cell density via weights</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistConstantICOp: Initialize particle distribution &amp; add SPDistConstantBCOp</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistDensityToFieldOp: Sum real and computational particles/cell to field</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistDSMCConstantBCOp: Injection of constant weight particles</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistESPushOp: Electrostatic particle push using node electric field</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistMoveOp: Linear particle push</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistPatchOp: Transfers particles between domains</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistSortOp: Sort particles according to cell ID</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistSplitOp: Split particle distribution into two by cell ID flag</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistToFieldOp: Sum particle charges to field entry</td>
</tr>
<tr>
<td>Plotting</td>
<td>LogicalFieldWrite1DOp: Write to output files for line plots</td>
</tr>
<tr>
<td>Plotting</td>
<td>LogicalFieldWriteVTKOp: Write to output files for 3D plots in .vts format</td>
</tr>
<tr>
<td>Plotting</td>
<td>LogicalFieldWriteVTKROp: Exports the field data in .vtr format</td>
</tr>
<tr>
<td>Plotting</td>
<td>LogicalVlasov2DWriterOp: Exports a 2D phase-space plot</td>
</tr>
<tr>
<td>Plotting</td>
<td>VlasovMetricsOp: Exports Vlasov metrics for mass and energy conservation</td>
</tr>
<tr>
<td>Plotting</td>
<td>VolumeRenderOp: Single cubic domain realtime volume rendering</td>
</tr>
<tr>
<td>Utility</td>
<td>CriteriaStageOp: Continue to next stage if quantity below criteria</td>
</tr>
<tr>
<td>Utility</td>
<td>NextStageOp: Continue to next stage</td>
</tr>
<tr>
<td>Vlasov</td>
<td>LogicalBCVlasovExtrapolateOp: Sets a velocity boundary conditions to extrapolation</td>
</tr>
<tr>
<td>Vlasov</td>
<td>LogicalVlasovCalcDensityOp: Calculates the density given a velocity distribution</td>
</tr>
<tr>
<td>Vlasov</td>
<td>LogicalVlasovCalcFluidVariablesOp: Calculate field variables given a velocity distribution</td>
</tr>
<tr>
<td>Vlasov</td>
<td>LogicalVlasovFluidBoltzmannSetOp: Boltzmann distribution initial condition for Vlasov fluid</td>
</tr>
<tr>
<td>Vlasov</td>
<td>LogicalVlasovFluidConstantICOp: Creates or initializes a new Vlasov fluid</td>
</tr>
<tr>
<td>Vlasov</td>
<td>Vlasov1DIVSLOp: Semi-Lagrangian Vlasov advection</td>
</tr>
<tr>
<td>Module</td>
<td>Operation</td>
</tr>
<tr>
<td>----------</td>
<td>------------------------------------------------</td>
</tr>
<tr>
<td>Field</td>
<td>BCFaceXtrapOp</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalBCMirrorMoveInOp</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalBCPeriodicOneDomOp</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalFieldAccumulateOp</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalGradientOp</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalICConstantOp</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalPoisonOp</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalPoisonStrip1DOp</td>
</tr>
<tr>
<td>Field</td>
<td>UFieldConstantICOp</td>
</tr>
<tr>
<td>Fluid</td>
<td>FluidConstantICOp</td>
</tr>
<tr>
<td>Fluid</td>
<td>FluidESPushOp</td>
</tr>
<tr>
<td>Fluid</td>
<td>FluidSphereICOp</td>
</tr>
<tr>
<td>Fluid</td>
<td>IntegrateFluxOp</td>
</tr>
<tr>
<td>Fluid</td>
<td>LinearSemiLagrangianOp</td>
</tr>
<tr>
<td>Fluid</td>
<td>RoeFluxCalc2Op</td>
</tr>
<tr>
<td>Fluid</td>
<td>RoeFluxCalcHLLE2Op</td>
</tr>
<tr>
<td>Fluid</td>
<td>RoeFluxCalcHLLEPOp</td>
</tr>
<tr>
<td>Fluid</td>
<td>RoeFluxCalcOp</td>
</tr>
<tr>
<td>Fluid</td>
<td>TVDFluxCalcOp</td>
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<tr>
<td>Geometry</td>
<td>LogicalMeshSurfaceSugarcubeOp</td>
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<tr>
<td>Geometry</td>
<td>SPDistBCSurfBoxICOp</td>
</tr>
<tr>
<td>Geometry</td>
<td>SPDistSugarcubeBCMoveOp</td>
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<tr>
<td>Geometry</td>
<td>SPDistSugarcubeSurfBCMoveOp</td>
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<tr>
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<td>SPDistBoxICOp</td>
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<td>Particle</td>
<td>SPDistBoxICOp</td>
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<td>SPDistDirectCellMergeOp</td>
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<tr>
<td>Particle</td>
<td>SPDistDirectCellSplitOp</td>
</tr>
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<td>Particle</td>
<td>SPDistESPhiCNPushOp</td>
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<tr>
<td>Particle</td>
<td>SPDistESPhiNCPushOp</td>
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<tr>
<td>Particle</td>
<td>SPDistESPhiNCNSpherePushOp</td>
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<td>Particle</td>
<td>SPDistESPhiPushOp</td>
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<td>Particle</td>
<td>SPDistMCCOp</td>
</tr>
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<td>Particle</td>
<td>SPDistPatchICOp</td>
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<tr>
<td>Particle</td>
<td>SPDistPerturbedCellIDOp</td>
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<tr>
<td>Particle</td>
<td>SPDistSortedStatToField4Dop</td>
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<tr>
<td>Particle</td>
<td>SPDistTemperatureToField4Dop</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistToEMField4Dop</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistToFieldLinear1Dop</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistToFieldLinear0p</td>
</tr>
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<td>Particle</td>
<td>SPDistVSortOp</td>
</tr>
<tr>
<td>Plotting</td>
<td>LogicalFieldStatWriteVTKOp</td>
</tr>
<tr>
<td>Plotting</td>
<td>LogicalFieldWriteVTKUOp</td>
</tr>
<tr>
<td>Plotting</td>
<td>LogicalVlasovFluidWrite1DProbeVDFOp</td>
</tr>
<tr>
<td>Plotting</td>
<td>UFieldWriteVTKOp</td>
</tr>
<tr>
<td>SourceModel</td>
<td>SPDistNormalMaxwellianStreamOp</td>
</tr>
<tr>
<td>Vlasov</td>
<td>LogicalBCPeriodicOneDomVlasovOp</td>
</tr>
<tr>
<td>Vlasov</td>
<td>LogicalFluidToLogicalVlasovFluidOp</td>
</tr>
<tr>
<td>Vlasov</td>
<td>LogicalVlasovFieldVolumeDomains</td>
</tr>
<tr>
<td>Vlasov</td>
<td>LogicalVlasovFluidSetOp</td>
</tr>
<tr>
<td>Vlasov</td>
<td>SPDistToLogicalVlasovFluidOp</td>
</tr>
</tbody>
</table>

Table 2. Summary of operations included in TURF-DEV.
### Table 3. Summary of additional experimental (E) and research (R) operations included in TURF-DEV.

<table>
<thead>
<tr>
<th>Module</th>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Field</td>
<td>ConstantAnnulusPotentialOp</td>
<td>(R) Apply annularly symmetric potential to field</td>
</tr>
<tr>
<td>Field</td>
<td>ConstantSphericalPotentialOp</td>
<td>(R) Apply spherically symmetric potential to field</td>
</tr>
<tr>
<td>Field</td>
<td>ConstantWellPotentialOp</td>
<td>(R) Apply constant parabolic well potential to field</td>
</tr>
<tr>
<td>Field</td>
<td>LogicalICFunctionOp</td>
<td>(E) Set field value using external function</td>
</tr>
<tr>
<td>Geometry</td>
<td>LogicalMeshSurfaceBBoxSplotchOp</td>
<td>(E) Mark surface triangle bounding box on cells</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistBCChildLangmuirOp</td>
<td>(E) Child Langmuir surface emission</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistBCSecondaryOp</td>
<td>(E) Secondary emission boundary condition</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistBCTransOp</td>
<td>(E) Translate particles in box to new location</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistCFEBCOp</td>
<td>(E) Fowler-Nordheim cold field emission BC</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistCopyPosBoxICOp</td>
<td>(E) Initialize particles with VDF but positions from second dist</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistESPhipushVerletHalfOp</td>
<td>(E) Verlet electrostatic potential particle push</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistDirectCellMergeMixOp</td>
<td>(R) Position from xv moment merge</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistDirectCellMergeMixXVOp</td>
<td>(R) Position from xv moment merge</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistDirectCellSplitMixOp</td>
<td>(R) Principal component analysis merge</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistDirectCellSplitMixXVOp</td>
<td>(R) Angular momentum preserving merge</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistDirectCellSplitPCAOp</td>
<td>(R) Principal component analysis split</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistDirectCellSplitXxXVOp</td>
<td>(R) Angular momentum preserving split</td>
</tr>
<tr>
<td>Particle</td>
<td>SPDistOrbiterICOp</td>
<td>(R) Period synchronized particle initial condition</td>
</tr>
<tr>
<td>Plotting</td>
<td>LogicalFieldCatalystOp</td>
<td>(E) Kitware Catalyst plotting connection</td>
</tr>
<tr>
<td>Utility</td>
<td>ConstantOperatorOp</td>
<td>(E) Work to allow generic constant parsing</td>
</tr>
<tr>
<td>Utility</td>
<td>FromGPUOp</td>
<td>(E) Recursive GSObject transfer from GPU</td>
</tr>
<tr>
<td>Utility</td>
<td>ToGPUOp</td>
<td>(E) Recursive GSObject transfer to GPU</td>
</tr>
<tr>
<td>Vlasov</td>
<td>CreateVlasovVariableOp</td>
<td>(E) Create new Vlasov fluid variable</td>
</tr>
<tr>
<td>Vlasov</td>
<td>LogicalVlasovFluidFunctionICOp</td>
<td>(E) Initialize Vlasov data using external function</td>
</tr>
<tr>
<td>Vlasov</td>
<td>SPDistConstantVlasBCOp</td>
<td>(R) Constant boundary conditions for VlasovPIC</td>
</tr>
<tr>
<td>Vlasov</td>
<td>SPDistConstantVlasICOp</td>
<td>(R) Constant initial conditions for VlasovPIC</td>
</tr>
<tr>
<td>Vlasov</td>
<td>SPDistVlas2wOp</td>
<td>(R) Density to weights for VlasovPIC</td>
</tr>
<tr>
<td>Vlasov</td>
<td>SPDistVlasDensityToFieldOp</td>
<td>(R) Integrate density to field data for VlasovPIC</td>
</tr>
<tr>
<td>Vlasov</td>
<td>SPDistw2VlasOp</td>
<td>(R) Weights to density for VlasovPIC</td>
</tr>
</tbody>
</table>
REFERENCES


1. Introduction

This tutorial provides steps in setting up the DSMC example provided in the following directory: tutorial-TURF/DSMC/DSMC\_1DShock. This folder contains two subfolders, DS1V and TURF. The DS1V contains reference cases for Argon shocks using the DS1V code described in Section 5 below. The TURF folder contains input files to run the same Argon shock cases within TURF. For example, the TURF/M1.2 folder contains the input files for running the Mach 1.2 shock test case. Once in the specific case directory, world.list should be pointed to the file world.dsmc1Dshock.list by typing

```
projects/dat-TURF/> ln -s world.dsmc1Dshock.list world.list
```

in the command line, as in other examples. The script file world.dsmc1Dshock.list will execute the DSMC operations listed in operations.dsmc1Dshock.list to simulate the 1D normal shock problem using the DSMC method. In order to run DSMC simulations properly, the value for FNUM must be set to the same value for all the DSMC operations, where FNUM is the number of physical particles represented by a single simulation particle. Therefore, when introducing particles into the domain, operations that require the user specified FNUM must be used; these operations are named as SPDistDSMCConstantICOp and SPDistDSMCConstantBCOp. The operation SPDistDSMCConstantICOp distributes particles uniformly inside the simulation domain. On the other hand, the operation SPDistDSMCConstantBCOp creates particles outside the domain, and a fraction of these particles flow into the domain. The DSMC collision calculation is done in SPDistDSMCOp, and the same FNUM used in the other operations must be used. Furthermore, SPDistDSMCSampleOp triggers the mixing of the field values between iterations, allowing a smoother distribution at the end of simulation. These DSMC operations are explained in this tutorial.
2. DESCRIPTION OF THE EXAMPLE PROBLEM

In a fluid, disturbance information is communicated within a medium at the speed of sound, allowing the upstream flow field to adjust accordingly. However, when the flow velocity is greater than the speed of sound, the disturbance information cannot be communicated fast enough, resulting in the formation of a shock. The shock creates a “discontinuity” or a sudden change in flow properties such as velocity, pressure, and temperature. Across a shock, the pressure and temperature always increase while the velocity always decreases from upstream to downstream.

The example to simulate with the DSMC part of TURF is the 1D normal shock problem, in which the shock forms in a plane perpendicular to the flow direction. In this problem, the flow properties at upstream and downstream regions with respect to the shock location are related through the following equations [3].

\[ \rho_1 u_1 = \rho_2 u_2 \]
\[ p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2 \]
\[ h_1 + \frac{1}{2} u_1^2 = h_2 + \frac{1}{2} u_2^2 \]

where \( \rho \) is the density, \( u \) is the velocity, \( p \) is the pressure, \( h \) is the enthalpy, and subscripts 1 and 2 denote upstream and downstream, respectively. Equation (1) is obtained by integrating the Euler equations, a set of conservation equations for mass, momentum, and energy that are applicable for such flows [1]. In a perfect gas, the speed of sound, \( a \), can be determined using the isentropic relation.

\[ a^2 = \left( \frac{\partial p}{\partial \rho} \right) = \frac{\gamma p}{\rho} = \gamma R_s T \]

where \( \gamma \) is the heat capacity ratio defined as \( \gamma = 1 + 2/f, f \) is the degree of freedom (i.e. 3 for a monatomic gas and 5 for a diatomic gas), \( R_s \) is the specific gas constant (i.e. 208.13 J/kg·K for argon), and \( T \) is the temperature. Using Eq. (1) and the perfect gas assumption, the downstream flow properties can be determined if the upstream flow properties are known [3].

\[ M_2^2 = 1 + \frac{\gamma - 1}{2} M_1^2 \]
\[ \frac{n_2}{n_1} = \frac{\rho_2}{\rho_1} = \frac{u_1}{u_2} = \frac{(\gamma + 1)M_1^2}{\gamma M_1^2 - 2} + \frac{1}{2} \]
\[ T_2 = 1 + \frac{2(\gamma - 1)}{(\gamma + 1)^2} \frac{\gamma M_1^2 + 1}{M_1^2} (M_1^2 - 1) \]

where \( M \) is the Mach number defined as \( M = u/a \) and \( n \) is the number density. In setting up the 1D normal shock problem, the downstream flow properties need to be evaluated and input in operations.list prior to running TURF.

3. SETTING UP THE DSMC EXAMPLE

One way to set up the 1D normal shock problem is to introduce uniformly distributed gases upstream and downstream of the shock location. Given the upstream flow properties, appropriate downstream flow properties are determined by Eqs. (3) to (5). Table 1 provides the downstream flow properties for argon gases of \( T_1 = 293 \), \( n_1 = 1 \times 10^{22} \) m\(^{-3}\), and \( q_1 = 318.8 \) m/s at \( M_1 \) of 1.2, 1.4, 2.0, and 8.0. The upstream flow velocities corresponding to the Mach number of 1.2, 1.4, 2.0, and 8.0 are 382.4, 446.2, 637.4, and 2549.6 m/s, respectively. In order to maintain the gas density and the shock location, the gas should also be flowing into the domain from the upstream boundary according to the flow 1. At the interface between the two gases at different flow properties, the properties are initially discontinuous, while they will develop smooth profiles as time evolves. These profiles can be compared with the profiles obtained by other DSMC models or fluid models. Examples of shock profiles are also provided in Ref. [2].

The script file world.dsmc1Dshock.list includes important parameters that define the problem, including the information related to computational grid, time-step, species, etc., as shown below. Referring to world.dsmc1Dshock.list, the number of interior cells can be found by dividing (bound_hi-bound_lo) by delta for each direction. In this example, the grid contains 1000 cells in x-direction and a single cell for both the y- and z-directions. The gas
Table 1. Downstream flow properties for upstream Mach number of 1.2, 1.4, 2.0, and 8.0. The values are for argon gas.

<table>
<thead>
<tr>
<th>Downstream Flow Property</th>
<th>Symbol</th>
<th>Unit</th>
<th>1.2</th>
<th>1.4</th>
<th>2.0</th>
<th>8.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity</td>
<td>$u_2$</td>
<td>m/s</td>
<td>294.9</td>
<td>282.3</td>
<td>278.9</td>
<td>667.3</td>
</tr>
<tr>
<td>Speed of Sound</td>
<td>$a_2$</td>
<td>m/s</td>
<td>348.4</td>
<td>376.0</td>
<td>459.4</td>
<td>1456</td>
</tr>
<tr>
<td>Mach Number</td>
<td>$M_2$</td>
<td></td>
<td>0.85</td>
<td>0.75</td>
<td>0.61</td>
<td>0.46</td>
</tr>
<tr>
<td>Number Density</td>
<td>$n_2$</td>
<td>1/m$^3$</td>
<td>$1.30 \times 10^{22}$</td>
<td>$1.58 \times 10^{22}$</td>
<td>$2.29 \times 10^{22}$</td>
<td>$3.82 \times 10^{22}$</td>
</tr>
<tr>
<td>Temperature</td>
<td>$T_2$</td>
<td>K</td>
<td>350.1</td>
<td>407.8</td>
<td>608.9</td>
<td>6116</td>
</tr>
</tbody>
</table>

species is argon. Furthermore, the parameters to be output are the number of computational and physical particles which are specified as $N_{Ar}$ and $C_{Ar}$, respectively. This example uses three stages: INITIALIZE, MOVE, and POSTOP. The script file operations.dsmc1Dshock.list contains all the operations within each of the three stages, as listed in Table 2. This tutorial only covers the DSMC operations including SPDistDSMCCConstantICOp, SPDistDSMCCConstantBCOp, SPDistDSMCOp, and SPDistDSMCSampleOp. Descriptions of the other operations can be found in other tutorials.

```
DEFINE WORLD
  NAME = DSMC_example
  op_file = operations.dsmc1Dshock.list
  coordinates = cartesian
  origin = (0.0,0.0,0.0)
  delta = (2.0e-5,2.0e-3,2.0e-3)
  end_time = 1.0e-4
  start_dt = 1.0e-8
  fields = [NAr, CAr]
  species = [Ar]
  stages = [INITIALIZE, MOVE, POSTOP]
  start_iteration = 0 # Number of Poisson Iteration Before Start
END WORLD

############################################################################
## Domain Geometry
############################################################################
DEFINE DOMAIN DOM000
  bound_lo = (0.0,0.0,0.0)
  bound_hi = (2.0e-2,2.0e-3,2.0e-3)
END DOMAIN

4. DSMC Operations

4.1. SPDistDSMCCConstantICOp. This operation sets up uniformly distributed particles within a box placed inside the simulation domain. An example of inputs for SPDistDSMCCConstantICOp are shown below. Unlike SPDistConstantICOp, the real to computational particle weight ratio, $F_{NUM}$, is specified as an input. The box to be filled with particles is bounded by $BOUND_{LO}$ and $BOUND_{HI}$, in which the lower and higher bounds in Cartesian coordinate are specified, respectively. The gas species is argon, and the corresponding mass of each molecule is 39.659 times the proton mass, $M_p$. In order to set up the 1D shock problem properly, the upstream and downstream regions inside the computational domain are filled with particles according to flow properties 1 and 2. The initial particle distribution obtained by the DSMC example is shown in Fig. 1. This example corresponds to the case with $M_1 = 1.2$, where the downstream flow properties are given in Table 1. Note that $N_{Ar}$ is related to the number
Table 2. Summary of operations listed in `operations.dsmc1Dshock.list`.

<table>
<thead>
<tr>
<th>Stage</th>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>INITIALIZE</td>
<td>SPDistDSMCCOnstantICOp</td>
<td>Initial distribution of particles inside the domain</td>
</tr>
<tr>
<td></td>
<td>SPDistConstantICOp</td>
<td>Null particle distribution in ghost cells</td>
</tr>
<tr>
<td>MOVEOP</td>
<td>SPDistDSMCCOnstantBCOp</td>
<td>Injection of particles</td>
</tr>
<tr>
<td></td>
<td>SPDistMoveOp</td>
<td>Advancement of particles</td>
</tr>
<tr>
<td></td>
<td>SPDistBCSpecOp</td>
<td>Specular boundary condition</td>
</tr>
<tr>
<td></td>
<td>SPDistCellIDOp</td>
<td>Find cell ID associated with particle location</td>
</tr>
<tr>
<td></td>
<td>SPDistSortOp</td>
<td>Sort particles according to cell ID</td>
</tr>
<tr>
<td></td>
<td>SPDistDSMCOp</td>
<td>DSMC collision calculation</td>
</tr>
<tr>
<td></td>
<td>LogicalFieldSetOp</td>
<td>Initialize the field parameters</td>
</tr>
<tr>
<td></td>
<td>SPDistDensityToFieldOp</td>
<td>Sum real and computational particles/cell to field</td>
</tr>
<tr>
<td>POSTOP</td>
<td>LogicalFieldWriteVTKOp</td>
<td>Write to output files for 3D plots</td>
</tr>
<tr>
<td></td>
<td>LogicalFieldWrite1DOp</td>
<td>Write to output files for line plots</td>
</tr>
</tbody>
</table>

Density $n$ such that $n = \frac{N_{Ar}}{\Delta V}$ where $\Delta V$ is the size of a cell in m$^{-3}$. There is a statistical noise associated with the number of computational particles as the particle locations are determined using the random number generator; the noise can be reduced by increasing the number of simulation particles.

```plaintext
DEFINE OPERATION
   TYPE = SPDistDSMCCOnstantICOp
   DATA_NAME = Ar-DST
   MAX_NP = 12800000
   BOUND_LO = (0.0,0.0,0.0)
   BOUND_HI = (1.0e-2,2.0e-3,2.0e-3)
   TEMPERATURE = 293.0
   Z = 0
   MASS = 39.659 Mp
   NUMBER_DENSITY = 1.0e22
   FNUM = 9.1892e8
   VEL = (382.447,0.0,0.0)
END OPERATION
```
4.2. **SPDistDSMCCConstantBCOp**. This operation sets up uniformly distributed particles within a box placed outside the simulation domain. The size of box is modified such that it lies within the ghost cell region. An example of inputs for **SPDistDSMCCConstantBCOp** are shown below. Similar to **SPDistDSMCCConstantICOp**, the box to be filled with particles is bounded by `BOUND_LO` and `BOUND_HI`.

In the DSMC example, particles flowing out the simulation domain from ±x boundaries are simply discarded, while fraction of particles created in the box flows into the simulation domain. When the simulation is at steady-state, the particle counts flowing in and out the domain are maintained to be nearly equal.

```plaintext
DEFINE OPERATION
    TYPE = SPDistDSMCCConstantBCOp
    DATA_NAME = Ar-DST
    TEMPERATURE = 293.0
    NUMBER_DENSITY = 1.0E22
    FNUM = 9.1892e8
    VEL = (382.447,0.0,0.0)
    BOUND_LO = (-0.01e-2, 0.0e-3, 0.0e-3)
    BOUND_HI = ( 0.00e-2, 2.0e-3, 2.0e-3)
END OPERATION
```

4.3. **SPDistDSMCOp**. This operation finds the number of collisions to perform within all the grid cells and apply collisions based on the DSMC method. The variable hard sphere (VHS) molecular model is used to determine the deflection of particles which requires inputs of `ALPHA` and `DIAM` where `ALPHA` and `DIAM` are the empirical factors that determine the diameter variation and reference diameter of the molecule, respectively. The `DIAM` is the reference molecular diameter at 273K such that a hard sphere of that diameter would have the correct fluid viscosity and
ALPHA is viscosity-temperature power law coefficient, \( \omega \), minus the hard sphere value of 0.5. It is important to note that ALPHA should not be confused with the variable soft sphere (VSS) model’s \( \alpha \) parameter. These parameters can be found in Ref. [2].

```plaintext
DEFINE OPERATION
  TYPE = SPDistDSMCOp
  SPDIST_DATA_NAME = Ar-DST
  MASS = 39.659 Mp
  ALPHA = 0.31
  FNUM = 9.1892e8
  KOVERM = 208.132
  DIAM = 4.17e-10
  FREQUENCY_TO_RESAMPLE_MFS = 2000
  SORT_OP_NAME = Sort_Ar-DST
END OPERATION
```

4.4. SPDistDSMCSampleOp. This operation is similar to SPDistDensityToFieldOp except that it starts to mix the fields after the time specified as an input. An example of inputs for SPDistDSMCSampleOp is shown below. In the DSMC example, the fields \( NAr \) and \( CNAr \) are computed from the particle distribution at the computational grid. After the time given to \( \text{MIX}_\text{START}\_\text{TIME} \), mixing between iterations is initiated. \( \text{MIX}_\text{START}\_\text{TIME} \) should be set to the time when the simulation becomes steady-state. This operation allows a smooth field distribution at the end of simulation without using a very large number of simulation particles. The field distributions at 2,000 and 10,000 time-steps are shown in Figs. 2 and 3, respectively. In this example, mixing has been performed after 8,000 time-steps; the distribution is smoothed out significantly after mixing the field parameters for the last 2,000 iterations.

```plaintext
DEFINE OPERATION
  TYPE = SPDistDSMCSampleOp
  FIELD_DATA_NAME = FieldData
  SPDIST_DATA_NAME = Ar-DST
  PSORT_NAME = Sort_Ar-DST
  FIELD_NAME = NAr CNAr
  MIX_START_TIME = 8.0e-5
END OPERATION
```

4.5. SPDistDSMCSample2Op. This operation is another version of SPDistDSMCSampleOp needed for long sampling times. Because TURF uses single precision floating point numbers for particles and fields for the sake of GPU performance, the direct DSMC sampling starts to lose accuracy for large numbers of samples. For the direct sample operation, the value of the sampled average field is first scaled by \( (n_{\text{sample}} - 1)/n_{\text{sample}} \) and then particle weights are accumulated into the sample average scaled by \( w_p/n_{\text{sample}} \). This means that in each cell, a number of order \( (\text{particles/cell}) * n_{\text{sample}} \) smaller than the total is added for each particle during the accumulation phase. At approximately \( O(1,000 - \text{particles/cell}) \) and \( O(10,000) \) samples, the added pieces are \( O(1e7) \) times smaller than the total resulting in lost single precision digits and bulk fluctuation of the sample values. Instead, the SPDistDSMCSample2Op uses two density buffers to help alleviate this issue, \( NAr \) and \( NbarAr \) (along with particle/cell counterparts). The instantaneous density is first accumulated in \( NAr \) using the standard SPDistDensityToFieldOp operation, and then the sample averaged value is updated via \( \bar{N}_{Ar} = (\bar{N}_{Ar} + (n_{\text{sample}} - 1)NAr)/n_{\text{sample}} \) for each cell. Furthermore, all calculations on the right hand side are performed in double precision prior to rounding to attempt to help retain as many digits of precision as possible during the calculation which is impossible with the sum updated in memory per particle as in the original version. The example shown also demonstrates the use of the LogicalFieldVolumetricMulOp to divide the value of \( NAr \) by the cell volume to convert absolute number of real particles per cell into number density. These modifications are not necessary for the simple tutorial versions of the
shock case because of the minimal sampling performed, but help in converging the results to the DS1V solution as part of the code verification process in the next section.

```
DEFINE OPERATION
  TYPE = SPDistDensityToFieldOp
  FIELD_DATA_NAME = FieldData
  SPDIST_DATA_NAME = Ar-DST
  FIELD_NAME = NAr CNAr # Computational and Physical Number per cell
END OPERATION

DEFINE OPERATION
  TYPE = LogicalFieldVolumetricMulOp
  DATA_NAME = FieldData
  FIELD_NAME = NAr
  OP_OPTION = DIV # Divide by Volume (Default is Multiply)
  RUN_AT_INIT = true
END OPERATION

DEFINE OPERATION
  TYPE = SPDistDSMCSample2Op
  FIELD_DATA_NAME = FieldData
  SPDIST_DATA_NAME = Ar-DST
  PSORT_NAME = Sort_Ar-DST
  SRC_FIELD_NAME = NAr CNAr # Instantaneous Computational and Physical Number/Cell
  DST_FIELD_NAME = NbarAr CNbarAr # Sampled Average Computational and Physical Number/Cell
  MIX_START_TIME = 8.0e-5
  SKIP = 5
END OPERATION
```
**Fig. 2.** Particle distribution after 2,000 steps.

**Fig. 3.** Particle distribution after 10,000 steps.
5. Comparison of Shock Profiles with Bird’s DSMC Code

The 1D shock profiles from the DSMC part of TURF can be compared with other DSMC programs for code verification; in this tutorial, the results are compared with the 1D DSMC code, DS1V, developed by G. A. Bird (available at www.gab.com.au). The DS1V code along with input files (ds1vd.dat) for the cases with \( M_1 = 1.2, 1.4, 2.0, \) and 8.0 are also provided in this tutorial. In order to obtain a smooth distribution at the end of simulation, DS1V is run twice; first, the simulation is started using the “new run” (#3) option in the terminal, the simulation is then stopped at a time greater than \( 2 \times 10^{-5} \) sec, and finally the simulation is restarted using “new sample” (#2) followed by the “adapt the cells” (#1) option. The resulting profile of density as a function of position can be extracted from the output file, “PROFILE.DAT.”

Figure 4 compares the shock profiles computed with TURF and DS1V for the upstream Mach number of 1.2 and 2.0. The values are normalized according to,

\[
\tilde{\rho} = \frac{\rho - \rho_1}{\rho_2 - \rho_1}
\]

The original profile obtained by TURF fluctuated considerably compared to the profile by DS1V when time averaged only over the last 20\( \mu s \) as shown in Figure 2. With the modification to the sampling procedure for 720\( \mu s \) of time averaging (similar to DS1V) as described in Section 4.5, Figure 4 show the agreement between the two programs is quite satisfactory.

**Fig. 4.** Normalized density computed by TURF and DS1V.

**References**

1. Introduction

The purpose of this tutorial is to provide information on the setup of the collisionless electrostatic shock test case. By this point it is assumed that you already have a basic understanding of how the operators in TURF work and the purpose of both the world.list and the various operations.*.list files. For a review of the purpose of these files please refer to the heatbath example tutorials. Instead this tutorial will focus on aspects that are specific to this simulation and will only provide a cursory overview of basic topics. This tutorial is divided up into three main sections, Section 2 provides an overview of the collisionless electrostatic shock experiment.

2. The Collisionless Electrostatic Shock

The collisionless electrostatic shock simulation is based on the experiment by Taylor, et.al, [2]. Figure 1 shows the experimental setup as planned for upcoming validation experiments at AFRL/RQRS including a pulse shape needed to drive a soliton used a related problem also originally performed in the same experimental device[1]. In this experiment, Argon gas is fully ionized and separated into driver and target sections of a vacuum chamber. The separation is maintained by a negatively biased grid held at a fixed potential. The number density of the driver side is higher then the target but they share the same ion and electron temperature. At the start of the experiment a ramp potential is applied to the driver side and a shock moves into the target side. For all cases the ion temperature and driven number density was held at 0.2 eV and $10^9$ cm$^{-3}$ respectively. A sweep of parameter space was accomplished by varying the electron temperature and the density of the driver gas. The electron to ion temperature varies between 6 and 20 while the density varies from 1 to 20 percent. The initial setup that saw the most study was at a density jump of 25 percent and an electron temperature of 7.5 and 15 eV.

There are several favorable parameters unique to this experiment that makes it an ideal test-case for a Vlasov-Poisson simulation.

- Ion-Ion collisions can be neglected because the mean-free-path between collisions is on the order of 300 Debye lengths ($\lambda_D$) and the total domain of the chamber is about $1000\lambda_D$.
- There are no applied magnetic fields and induced currents can be assumed to be negligible which obviate the need to solve the full Maxwell equations.
- The spatial symmetries of the experiment limit variations to be in only one direction so that a 1D1V Vlasov simulation of the flow is sufficient.

In addition to these parameters, several additional assumptions are made which will be tested throughout the upcoming TURF code validation and verification campaign.

- Modeling ion kinetic effects is important due to the collisionless nature of the plasma. This is to be validated through comparison of kinetic and fluid solutions.
The electrons can be accurately modeled as a Boltzmann equilibrium fluid so that the fastest time scale that needs to be resolved is the ion plasma frequency. This will be tested through comparison with experimental results as well as future fully kinetic simulations which include electron kinetic effects.

The flow is robust against spontaneously generated transverse modes so that the one-dimensional character of the flow is preserved far enough from the boundaries.

Fig. 1. Design of AFRL/RQRS double plasma device experiments.

- Pulse $\rightarrow$ Soliton
- Ramp $\rightarrow$ Shock

References


1. Introduction

The purpose of this tutorial is to provide an overview of how to setup and run a Vlasov simulation in the Thermophysics Universal Research Framework (TURF). By this point it is assumed that you already have an basic understanding of how the operators in TURF work and the purpose of both the world.list and the various operations.*.list files. For a review of the purpose of these files please refer to the heatbath example tutorials. Instead this tutorial will focus on aspects that are specific to this simulation and will only provide a cursory overview of basic topics. This tutorial is divided up into three main sections: Section 1 of this tutorial provides an overview of the collisionless electrostatic shock experiment, Section 2 provides an explination of the world.list file, and finally Section 3 details the operators necessary to run the collisionless electrostatic shock simulation with the Vlasov solver within TURF.

2. World.list

The world.list file defines important parameters that are not unique to any one particular operator. This includes information about the mesh, the time step and total run time, as well as the global variables. The only new information included in the world.list that is unique to Vlasov solvers is the definition of the velocity space origin and mesh spacing. These variables are defined via:

```
velocity_origin = (0.0,-0.5,-0.5)
velocity_delta = (15.625,1.0,1.0)
```

At this time each species can have its own unique bounds in velocity space but they must share the same mesh spacing and origin.

This simulation uses seven different field variables including the electron and ion densities, the electric field vector, the electric potential, a density for the electric field solver, mean Velocity, and temperature and are defined:

```
fields = [rhoE, rhoI, Ex, Ey, Ez, phi, rho_source]
fields = [Vmeanx, Vmeany, Vmeanz, Temperature]
```
3. operations.vlasov.list

This section explains how to solve this problem using Vlasov methods within TURF. It is assumed that the reader has a basic understanding of how to setup a simulation in TURF and only the information relevant to Vlasov and this simulation in particular are detailed. The operations.vlasov.list file are broken up into three stages, INIT, MOVE, and POSTOP which are responsible for the initialization, solvers, and plotting respectively.

3.1. operations.vlasov.list Initialization. In the initialize stage it is necessary to set the initial conditions which includes defining a new phase-space variable. The phase space variable, \( f_{\text{Ar}^+} \), is defined using:

```
DEFINE OPERATION
  TYPE = CreateVlasovVariableOp
  DATA_NAME = VlasovFluidData
  VBOX_LO = (-6000.0, -0.5, -0.5)
  VBOX_HI = ( 6000.0, 0.5, 0.5)
  VBOX_NGHOST = [3 0 0]
  SPECIES_NAMES = fAr+
  SPECIES_COMPOSITION = Ar
END OPERATION
```

The different fields are relatively self explanatory, but it should be noted that \( VBOX_{LO/HI} \) are in units of meters per second and the unused dimensions, \( V_y \) and \( V_z \), need to have a length of one. Another important parameter is the \( \text{VBOX\_NGHOST} \) which set the number of ghost cells in each velocity direction. If left unset, the default value of 3 ghost cells in the unused direction increases memory requirements by a factor of 49. The variable name is defined in \( \text{SPECIES\_NAMES} \), multiple species can be defined in this field. At a minimum the solver needs to know the mass and charge of each species. This is accomplished in one of two ways. The preferred method is to define the individual species that makes up each \( \text{SPECIES\_NAMES} \). This is defined in \( \text{SPECIES\_COMPOSITION} \). \( \text{SPECIES\_COMPOSITION} \) will parse a chemical formula and calculate its mass and charge using an internal database of elements. Any values defined in \( M \) and \( Z \) will be ignored. The second method is to manually set the mass and charge via \( M \) in kg and \( Z \) respectively. For this method to work you must set the \( \text{SPECIES\_COMPOSITION} \) to None. These two methods can be used together, but place holder will be needed in \( M \) and \( Z \) for the species defined via their \( \text{SPECIES\_COMPOSITION} \). For example the following code will use the internal database to calculate the mass and charge of \( f_{\text{Ar}^+} \) and \( f_{\text{Ar}} \) but will set \( \text{FakeVar} \) using the values in \( M \) and \( Z \). Note that place holders in \( M \) and \( Z \) are required.

```
SPECIES_NAMES = fAr+, FakeVar, fAr
SPECIES_COMPOSITION = Ar, None, Ar
M = -1.0, 1.0e-12, 23.3
Z = 1, -2, 0
```

This operator will not set the initial value of \( f_{\text{Ar}^+} \) so we will need to call another operator to set the distribution. This is accomplished by:

```
DEFINE OPERATION
  TYPE = LogicalVlasovFluidBoltzmannSetOp
  PHASESPACE_TYPE = VlasovFluidData
  BOUND_LO = (-100.0e-3, -0.5, -0.5)
  BOUND_HI = ( 0.0e-3, 0.5, 0.5)
  PHASESPACE_NAME = fAr+
  TEMPERATURE_K = 2320.8 # 1.5ev
  NUMBER_DENSITY = 1.25e15
  INIT_ONLY = true
  NUMBER_OF_DIMENSIONS = 1
END OPERATION
```

This sets up the initial VDF with a Boltzmann distribution for the driver side. The target side is set using the same operator but with different \( \text{BOUND\_LO/HI} \) values and density. The important parameters are \( \text{TEMPERATURE\_K} \).
and NUMBER DENSITY which sets the temperature in Kelvin and the total number density per cell in m⁻³. It should be noted that the molecular mass does not need to be defined because that information is stored within the variable fAr+. Another important parameter is INIT_ONLY which tells the operator that it should only run once at the beginning of the simulation. Otherwise the operation will overwrite the update with the initial conditions, though this could also be used as Dirichlet boundary condition at domain edges in other simulations.

3.2. operations.vlasov.list Move. The next stage to run is the MOVE stage. This stage contains the advection of the fluid in phase space as well as the electric field solver and is broken up into four main steps: (1) X-advection (half ∆t), (2) Electric field solver, (3) Vₚ-advection (full ∆t), (4) X-advection (half ∆t). This dimensionally split procedure was originally developed for the Vlasov equation by Cheng and Knorr and provides a second order integration in time[1]. The advection in phase space uses a Semi-Lagrangian method with WENO style interpolation and was developed by Qiu and Christlieb[2]. This method was chosen because it was found to be an accurate and efficient solver. The X-advection consists of two different operations, the first sets the ghost cells while the second advects the fluid in the X direction.

```plaintext
DEFINE OPERATION
  TYPE = LogicalBCVlasovExtrapolateOp
  NAME = PeriodicBCX1
  DATA_NAME = VlasovFluidData
  FIELD_NAME = fAr+
  DIRECTION = X
END OPERATION

DEFINE OPERATION
  TYPE = Vlasov1D1VSLOp
  NAME = Vlasov1D1VSL_X1
  DIRECTION = X
  VARIABLE_NAME = fAr+
  TIME_SCALE = 0.5
  VARIABLE_TYPE = VlasovFluidData
END OPERATION
```

It should be noted that TIME SCALE is set to 0.5 which indicates that only a half time step should be taken.

The next set of operations are used to calculate the electric field using Boltzmann equilibrium electrons. Many of the variables are self explanatory but one parameter, RUN_AT_INIT, needs further explanation. RUN_AT_INIT signifies that the apply function of the operator should also be run during the initialization stage. Typically, during the initialization stage the operator will only parse the input file, create the required memory, and if necessary set the initial conditions. In most cases this is enough, but some variables, such as the electric field, its value is not explicitly known and a routine must be used to calculate it. Since the method used to calculate the initial electric field is the same used during the simulation it is more practical to define these operators once during the MOVE stage and set the RUN_AT_INIT to true.

```plaintext
DEFINE OPERATION
## Calculates several useful field variables from a velocity distribution
## including density, mean velocity and temperature. This routine may be used
## instead of LogicalVlasovCalcDensityOp
  TYPE = LogicalVlasovCalcFluidVariablesOp
  NAME = CalcFluidVariables
  PHASESPACE_TYPE = VlasovFluidData
  PHASESPACE_NAME = fAr+
  DENSITY_TYPE = FieldData
  DENSITY_NAME = rho_tmp
  MEAN_V_PREFIX = Vmean
  TEMPERATURE_NAME = Temperature
END OPERATION
```

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**DEFINE OPERATION**

## Calculates Density by integrating over velocity space

- **TYPE**: LogicalVlasovCalcDensityOp
- **PHASESPACE_TYPE**: VlasovFluidData
- **PHASESPACE_NAME**: fAr+
- **DENSITY_TYPE**: FieldData
- **DENSITY_NAME**: rhoI
- **RUN_AT_INIT**: true

**END OPERATION**

**DEFINE OPERATION**

## Sets electric potential (phi) to zero

- **TYPE**: LogicalFieldSetOp
- **DATA_NAME**: FieldData
- **VALUE**: 0.0
- **FIELD_NAME**: phi
- **INIT_ONLY**: false
- **RUN_AT_INIT**: true

**END OPERATION**

**DEFINE OPERATION**

## Add electron and ion density

- **TYPE**: LogicalFieldAddOp
- **DATA_NAME**: FieldData
- **FIELD_SRCB_NAME**: rhoE
- **FIELD_SRCC_NAME**: rhoI
- **FIELD_DST_NAME**: rhoE
- **RUN_AT_INIT**: true

**END OPERATION**

**DEFINE OPERATION**

## Multiples the ion density by the mass of an electron to convert from number density to mass density and set to rho_source

- **TYPE**: LogicalFieldScalarMulOp
- **DATA_NAME**: FieldData
- **FIELD_SRC_NAME**: rhoI
- **FIELD_DST_NAME**: rho_source
- **SCALAR**: 1.602189200e-19
- **RUN_AT_INIT**: true

**END OPERATION**

**DEFINE OPERATION**

## Finds mass of ions in each cell, i.e., no longer density

- **TYPE**: LogicalFieldVolumetricMulOp
- **DATA_NAME**: FieldData
- **FIELD_NAME**: rho_source
- **RUN_AT_INIT**: true

**END OPERATION**
### Sets Electric field boundary conditions on the left hand side

```
TYPE = LogicalBCXtrap
NAME = Neumann-X-
DATA_NAME = FieldData
FIELD_NAME = phi
BOUND_LO = (-120.0e-3, -1.0, -1.0)
BOUND_HI = (-95.0e-3, 1.0, 1.0)
```

### Sets Electric field boundary conditions on the right hand side

```
TYPE = LogicalBCConstantOp
NAME = Electrode-X+
value = 0.0 #
DATA_NAME = FieldData
FIELD_NAME = phi
BOUND_LO = (95.0e-3, -1.0, -1.0)
BOUND_HI = (120.0e-3, 1.0, 1.0)
```

### Finds the electric field from the gradient of the electric potential and multiplies by a constant

```
TYPE = LogicalGradientCellCenterOp
FIELD_DATA_NAME = FieldData
FIELD_POTENTIAL_NAME = phi
FIELD_GRADIENT_PREFIX = E
FIELD_MULTIPLY_CONSTANT = -2.415365e6 # ec/(MW*amu) -2.415365e6
FIELD_GRADIENT_DIRECTIONS = [x, y, z] ## Ex,Ey,Ez
RUN_AT_INIT = true
BOUNDARY_TYPE = EXTRAPOLATE
```

The $V_x$-advection consists of two different operations, the first sets the ghost cells while the second advects the fluid in the $V_x$ direction.

```
TYPE = LogicalBCVlasovExtrapolateOp
NAME = PeriodicBCY
```
The final step of the MOVE stage is the second advection in the $X$-direction, which uses the same two operations used before.

The third and final stage is the POSTOP stage. This stage is responsible for preparing and saving the results to various output files.

The first output file is a two-dimensional phase-space plot. The purpose of this operator is to take any two dimensions, $X, Y, Z, V_x, V_y,$ or $V_z$ and a coordinate in phase space and slice along those planes. This is controlled by the following variables, $SPACE_CORD, VELOCITY_CORD, X_PLOT_DIRECTION,$ and $Y_PLOT_DIRECTION$ which sets the spatial coordinate, phase space coordinate the coordinate to plot along the “$X$” axis and the phase space coordinate to plot along the “$Y$” axis respectively. This operator looks like:
The next plotting operator is a bit of a hack and could be changed in future releases. The operator is designed to save the spatial data, e.g., density, electric field, and it is desirable to use the same operator regardless of the number of spatial dimensions. Unfortunately the VTK file format does not have a convenient mechanism to save one-dimensional data. To get around this an additional parameter \texttt{SAVE\_AS\_CSV} was added that saves the data in csv file format rather than the standard VTR format. The operator is set via:

```
DEFINE OPERATION
  TYPE = LogicalFieldWriteVTKROp
  DATA\_NAME = FieldData
  FILE\_HEAD = shockdata/field_data
  FIELD\_NAME = rhoI, phi, Ex, rho\_source, Vmeanx, Vmeany, Vmeanz, Temperature, Ne-
  SKIP = 2
  DIMENSIONS = 2
  nFIELD\_NAME = 4
  RUN\_AT\_INIT = true
  SAVE\_AS\_CSV = true
END OPERATION
```

The final operator in this stage is used to save various metrics including the density, energy, entropy and electric field norms over time. The operator is set up via:

```
DEFINE OPERATION
  TYPE = VlasovMetricsOp
  PHASESPACE\_TYPE = VlasovFluidData
  SPACE\_TYPE = FieldData
  PHASESPACE\_NAME = fAr+
  DENSITY\_NAME = rhoI
  E\_FIELD\_PREFIX = E
  E\_FIELD\_DIRECTIONS = [x, y, z]
  FILE\_NAME = shockdata/norms.csv
  SKIP = 1
  RUN\_AT\_INIT = true
END OPERATION
```
4. Appendix

Table 1. Summary of operations listed for the collisionless shock Vlasov example.

<table>
<thead>
<tr>
<th>Stage</th>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>INITIALIZE</td>
<td>CreateVlasovVariableOp</td>
<td>Create a Vlasov variable</td>
</tr>
<tr>
<td></td>
<td>LogicalVlasovFluidBoltzmannSetOp</td>
<td>Sets initial conditions of a Vlasov variable using a Boltzmann distribution</td>
</tr>
<tr>
<td>MOVE</td>
<td>LogicalVlasovCalcFluidVariablesOp</td>
<td>Calculate field variables given a velocity distribution</td>
</tr>
<tr>
<td></td>
<td>LogicalBCVlasovExtrapolateOp</td>
<td>Sets a velocity boundary conditions to extrapolation, i.e. simple non-reflecting</td>
</tr>
<tr>
<td></td>
<td>Vlasov1D1VSLOp</td>
<td>Advecets a Vlasov variable using the Semi-Lagrangian method</td>
</tr>
<tr>
<td></td>
<td>LogicalVlasovCalcDensityOp</td>
<td>Calculates the density given a velocity distribution</td>
</tr>
<tr>
<td></td>
<td>LogicalFieldSetOp</td>
<td>Set field values to constant</td>
</tr>
<tr>
<td></td>
<td>LogicalFieldAddOp</td>
<td>Adds one field variable to another</td>
</tr>
<tr>
<td></td>
<td>LogicalFieldScalarMulOp</td>
<td>Multiplies field by scalar constant</td>
</tr>
<tr>
<td></td>
<td>LogicalFieldVolumetricMulOp</td>
<td>Multiplies or divides field data by cell volumes</td>
</tr>
<tr>
<td></td>
<td>LogicalBCXtrapOp</td>
<td>Sets a physical boundary to extrapolation</td>
</tr>
<tr>
<td></td>
<td>LogicalBCConstantOp</td>
<td>Sets a physical boundary to be a constant</td>
</tr>
<tr>
<td></td>
<td>LogicalPoissonBoltzmannStrip1DOp</td>
<td>Solves for the electric field assuming a Boltzmann electron</td>
</tr>
<tr>
<td>POSTOP</td>
<td>LogicalGradientCellCenterOp</td>
<td>Calculates the gradient of a field vector</td>
</tr>
<tr>
<td></td>
<td>LogicalVlasov2DWriterOp</td>
<td>Exports a 2D phase-space plot</td>
</tr>
<tr>
<td></td>
<td>LogicalFieldWriteVTKROp</td>
<td>Exports the field data, e.g., density, velocity,...</td>
</tr>
<tr>
<td></td>
<td>VlasovMetricsOp</td>
<td>Exports Vlasov metrics data e.g., mass and energy conservation</td>
</tr>
</tbody>
</table>

References


1. INTRODUCTION

This tutorial demonstrates running a simple 3D electrostatic particle in cell (PIC) case in the Thermophysics Universal Research Framework (TURF). This tutorial assumes familiarity with the simple heatbath tutorials. New users are referred to those tutorials for further explanation. The TURF input files can be located in tutorial-TURF/GroundedBox/ES-PIC. You should see several files with the .list extension, which act as the scripting files for TURF.

The grounded box test case was developed to verify TURF’s PIC algorithms with respect to AFRL/RD’s ICEPIC particle in cell code running in electrostatic PIC mode [1]. The initial conditions are a uniform unit meter cube of zero velocity protons at a density of 1e10/m^3. In one octant of the cube, the proton charge is neutralized with 1e10/m^3 electrons with neither velocity nor thermal velocity. The walls of the cube are set to a fixed 0-Volt potential. The electrons are then accelerated by the field due to the charge of the non-neutralized protons in the remaining 7 octants of the box. The field evolves as the electrons accelerate such that the cloud oscillates and evolves within the box. Particles that hit the edge of the box are assumed to be neutralized and removed from the simulation.

Date: 1/31/2015.
2. WORLD.list

Running the TURF executable in the working directory will have TURF search for the default script file, `world.list`, and parses it automatically. We can take a look at the script by opening the file. The first block that defines the WORLD is shown below.

```plaintext
DEFINE WORLD
   NAME = ICEPIC-Bench
   op_file = operations.list
   coordinates = cartesian
   origin = (0.0,0.0,0.0)
   delta = (0.02,0.02,0.02)
   end_time = 10.0e-6
   start_dt = 2.50e-9
# Names Should not be fully contained in an earlier name for Plotting
   fields = [rho, Enx, Eny, Enz, phi, residual_phi, Np+, Ne-, CNp+, CNe-]
   stages = [INITIALIZE, SOLVE, MOVE, PLOT]
END WORLD
```

The options defined in this file should look familiar after completing the heatbath tutorial. In this example, the world is named “ICEPIC-Bench” to denote that it was originally intended to serve as a benchmark verification run against the ICEPIC code. The sample uses the `operations.list` operations file to define the simulation algorithm which will be discussed below. The remainder of the world definition sets a global cartesian coordinate system with 2\( \text{cm} \) cells along with 2.5\( \text{ns} \) time steps up to a final simulation time of 10\( \mu \text{s} \). The next line defines 10 field variables for charge density (\( \rho \)), 3 node centered electric field components (\( \text{En} \)), the electrostatic potential (\( \phi \)), an auxiliary variable for calculating the residual of the potential during the field solve (\( \text{residual\_phi} \)), and proton and electron physical and computational particle counts in cells (\( \text{Np+}, \text{Ne-}, \text{CNp+}, \text{CNe-} \)).

The example run is broken into 4 stages named INITIALIZE, SOLVE, MOVE, and PLOT. The two additional stages compared to the heatbath example are to accommodate an iterative electrostatic potential solve stage (SOLVE) and to ensure synchronization prior to the plotting operation stage (PLOT) though the later is not strictly necessary.

The last section of `world.list` defines the active domain for the simulation. In this example, it is simply a 1\( \text{m} \) unit cube starting from the coordinate origin. Using the global mesh spacing of 2\( \text{cm} \) from the WORLD definition results in a 50x50x50 active cell cube with the default 3 “ghost”-cells added to the high and low side in each direction for application of boundary conditions.

```plaintext
### Domain Geometry
#### DEFINE DOMAIN DOM000
   bound_lo = (0.0,0.0,0.0)
   bound_hi = (1.0,1.0,1.0)
END DOMAIN
```
3. operations.list

In this tutorial, the operations file will be considered in stages.

3.1. INITIALIZE. This stage creates new particle electron and proton particle distributions. The SPDistConstantICOp operation should be familiar from the heatbath example. Notable differences are that the charges, \( Z \), are non-zero and the electron mass is defined in units of electron mass instead of proton mass.

```plaintext
DEFINE STAGE INITIALIZE

####################################################################
## Initial Particle Distributions and Ghost/Exchange Distributions ##
####################################################################

DEFINE OPERATION
    TYPE = SPDistConstantICOp
    DATA_NAME = e-DST
    MAX_NP = 2000000
    FILL_RATIO = 1.0 #4.0
    BOUND_LO = (0.0,0.0,0.0)
    BOUND_HI = (0.5,0.5,0.5)
    temperature = 0.0 #11604.5059 # 1ev
    number_density = 1.e10
    Z = -1
    Mass = 1.0 Me
    vel = (0.,0.,0.)
END OPERATION

DEFINE OPERATION
    TYPE = SPDistConstantICOp
    DATA_NAME = p+DST
    FILL_RATIO = 0.0625
    MAX_NP = 2000000
    BOUND_LO = (0.0,0.0,0.0)
    BOUND_HI = (1.0,1.0,1.0)
    temperature = 0.0 #11604.5059 # 1ev
    number_density = 1.e10
    Z = 1
    Mass = 1.0 Mp
    vel = (0.,0.,0.)
END OPERATION

Next, empty “ghost” particle distributions are created again using SPDistConstantICOp. These are empty buffers where particles that have escaped the domain get copied later on in the sort.

```
The next set of operations sort the particles by the cell in which they reside. Though still part of the “INITIALIZE” stage, they will run every time the simulation loops back through that stage. The SPDistCellIDOp operation identifies which cell the particle resides in and saves it to the “CellID” variable within the particle distribution. The SPDistSortOp operation sorts the particles by their “CellID” and any particle that has escaped the domain gets separated into the ghost distribution.

```operation
DEFINE OPERATION
    TYPE = SPDistCellIDOp
    DATA_NAME = e-DST
END OPERATION

DEFINE OPERATION
    TYPE = SPDistCellIDOp
    DATA_NAME = p+DST
END OPERATION

DEFINE OPERATION
    TYPE = SPDistSortOp
    NAME = Sort_e-DST
    SRC_NAME = e-DST
    DST_NAME = e-GST
END OPERATION

DEFINE OPERATION
    TYPE = SPDistSortOp
    NAME = Sort_p+DST
    SRC_NAME = p+DST
    DST_NAME = p+GST
END OPERATION
```

The next sections accumulates particle quantities into the cell field variables. Before the data can be accumulated, the field variables must be cleared using the LogicalFieldSetOp. In future version of TURF, these operations may be optionally fused, but the separate combination is more general. The actual accumulation of field data is performed by the SPDistDensityToFieldOp and SPDistToFieldOp. The first is used to set diagnostic fields for number of real (Nₓ) and computational (CNₓ) particles per cell. It is worth noting that these numbers are both raw sums. To obtain the density, “n” from N, a LogicalFieldVolumetricMulOp. This usage can be seen in the Vlasov collisionless shock tutorial. The second operation multiples by particle charge while doing the accumulation such that the charge density is computed. More computationally efficient calculations can now be performed using field multiplication and summation operations, but the example in this tutorial was created using an early version of TURF that existed before those operations had been completed. This functionality can also be seen in the Vlasov collisionless shock tutorial.

```operation
DEFINE OPERATION
    TYPE = SPDistDensityToFieldOp
    SRC_NAME = e-DST
    DST_NAME = e-N
    DST_NAME = e-CN
END OPERATION

DEFINE OPERATION
    TYPE = SPDistToFieldOp
    SRC_NAME = p+DST
    DST_NAME = p+Nu
END OPERATION
```
DEFINE OPERATION
  TYPE = LogicalFieldSetOp
  DATA_NAME = FieldData
  FIELD_NAME = CNe-
  VALUE = 0.0
END OPERATION

DEFINE OPERATION
  TYPE = LogicalFieldSetOp
  DATA_NAME = FieldData
  FIELD_NAME = CNp+
  VALUE = 0.0
END OPERATION

DEFINE OPERATION
  TYPE = LogicalFieldSetOp
  DATA_NAME = FieldData
  FIELD_NAME = Ne-
  VALUE = 0.0
END OPERATION

DEFINE OPERATION
  TYPE = LogicalFieldSetOp
  DATA_NAME = FieldData
  FIELD_NAME = Np+
  VALUE = 0.0
END OPERATION

# Accumulate
DEFINE OPERATION
  TYPE = SPDistDensityToFieldOp
  FIELD_DATA_NAME = FieldData
  SPDIST_DATA_NAME = e-DST
  PSORT_NAME = Sort_e-DST
  FIELD_NAME = Ne- CNe- # Computational and Physical Number per Cell
END OPERATION

DEFINE OPERATION
  TYPE = SPDistDensityToFieldOp
  FIELD_DATA_NAME = FieldData
  SPDIST_DATA_NAME = p+DST
  PSORT_NAME = Sort_p+DST
  FIELD_NAME = Np+ CNp+ # Computational and Physical Number per Cell
END OPERATION

DEFINE OPERATION
  TYPE = LogicalFieldSetOp
  DATA_NAME = FieldData
  FIELD_NAME = rho

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\[\text{VALUE} = 0.0\]

\text{END\ OPERATION}

\text{DEFINE\ OPERATION}
\begin{verbatim}
  TYPE = SPDistToFieldOp
  FIELD\_DATA\_NAME = FieldData
  SPDIST\_DATA\_NAME = e-DST
  FIELD\_NAME = rho
\end{verbatim}

\text{END\ OPERATION}

\text{DEFINE\ OPERATION}
\begin{verbatim}
  TYPE = SPDistToFieldOp
  FIELD\_DATA\_NAME = FieldData
  SPDIST\_DATA\_NAME = p+DST
  FIELD\_NAME = rho
\end{verbatim}

\text{END\ OPERATION}

Finally, the “INITIALIZE” stage is completed with the \text{NextStageOp} operation to proceed to the “SOLVE” stage.

\text{DEFINE\ OPERATION}
\begin{verbatim}
  # Default Criteria to Proceed to the Next Stage
  TYPE = NextStageOp
\end{verbatim}

\text{END\ OPERATION}

\text{END\ STAGE\ INITIALIZE}

###

3.2. SOLVE. This stage iterates on solving for the electrostatic potential until the residual is small enough to proceed. The first step of the iterative field solve is to set the boundary condition potential to 0 on all six faces of the box. This is done using the \text{LogicalBCConstantOp} operation. The operation is relatively straightforward. The \(\phi\) variable of the default \text{FieldData} object is set to a potential of 0 Volts inside of the box defined by \text{BOUND}\_LO and \text{BOUND}\_HI. In this configuration of TURF, the potential is assumed to be cell centered. More specifically, the potential is set to 0 for every cell which has a cell center inside the physically defined box. This may lead to errors on the order of \(\Delta x\) on the location of the application of the boundary condition, but with the boundary conditions defined physically, the solution should converge to the exact solution with grid refinement without manual reconfiguration of the operations. This same approach is used when creating the domains which snap to the nearest approximation of cells based on the physical constraints independent of the underlying mesh resolution. Once again, the \text{NAME} variable for the operation is simply a designator label for output readability and the value in the \text{NAME} is not evaluated by the code to influence application of the operation. Boundary condition boxes are chosen to be large enough to contain at a minimum the first few layers of cell centers even at the coarsest resolutions run. In regions where the physical boundary conditions overlap, the value will be set repeatedly.

###

\text{DEFINE\ STAGE\ SOLVE}

\text{DEFINE\ OPERATION}
\begin{verbatim}
  TYPE = LogicalBCConstantOp
  NAME = Electrode-X-
  DATA\_NAME = FieldData
  FIELD\_NAME = \phi
\end{verbatim}
VALUE = 0.0 #
BOUND_LO = (-0.1,-0.1,-0.1)
BOUND_HI = (0.0,1.1,1.1)
END OPERATION

DEFINE OPERATION
  TYPE = LogicalBCConstantOp
  NAME = Electrode-X+
  VALUE = 0.0 #
  DATA_NAME = FieldData
  FIELD_NAME = phi
  BOUND_LO = (1.0,-0.1,-0.1)
  BOUND_HI = (1.1,1.1,1.1)
END OPERATION

DEFINE OPERATION
  TYPE = LogicalBCConstantOp
  NAME = Electrode-Y+
  VALUE = 0.0 #
  DATA_NAME = FieldData
  FIELD_NAME = phi
  BOUND_LO = (-0.1,1.0,-0.1)
  BOUND_HI = (1.1,1.1,1.1)
END OPERATION

DEFINE OPERATION
  TYPE = LogicalBCConstantOp
  NAME = Electrode-Y-
  VALUE = 0.0 #
  DATA_NAME = FieldData
  FIELD_NAME = phi
  BOUND_LO = (-0.1,-0.1,-0.1)
  BOUND_HI = (1.1,0.0,1.1)
END OPERATION

DEFINE OPERATION
  TYPE = LogicalBCConstantOp
  NAME = Electrode-Z+
  VALUE = 0.0 #
  DATA_NAME = FieldData
  FIELD_NAME = phi
  BOUND_LO = (-0.1,-0.1,1.0)
  BOUND_HI = (1.1,1.1,1.1)
END OPERATION

DEFINE OPERATION
  TYPE = LogicalBCConstantOp
  NAME = Electrode-Z-
  VALUE = 0.0 #
  DATA_NAME = FieldData
  FIELD_NAME = phi
  BOUND_LO = (-0.1,-0.1,-0.1)
  BOUND_HI = (1.1,-0.1,-0.1)
After the boundary conditions have been set, the actual Poisson solve can be performed. Currently, the set of elliptic solvers in TURF is relatively minimal and includes only red-black Gauss-Seidel and tri-diagonal ADI-type solvers as indicated below by the `LogicalPoissonStripOp` operation. There is also degenerate 1D version of the solver that can be used in fundamentally 1D problems or as an accelerated initial guess for solutions that are primarily one dimensional. The only non-default options for the solver selected were to not cycle sweep directions and to sub-cycle the operation 3 times before continuing. The operation is also applied in a red-black checkerboard in the iterative directions so that the solution is independent of the order in which the line relaxation sweeps are performed.

The last part of the `SOLVE` stage is defining the criteria to iterate the stage or continue to the next. First, the residual of \( \phi \) is computed in every cell and stored in \( \text{residual}_\phi \) using the `LogicalResidualOp` operation. The `LogicalNormOp` operation calculates the norm of the residual. The `NORM` parameter defines the power \( p \) for any \( L^p \)-norm. The operation creates a new scalar variable \( \text{SUMresidual}_\phi \_L2.00e+00 \) based off the name of the field in which the residual resides and the power of the norm to store the accumulated total residual. Finally, the `CriteriaStageOp` evaluates whether the summed residual is below the required threshold `CRITERIA`. Each domain applies this operation independently. At the end of each stage, every process collects one vote from every domain as to whether or not to proceed to the next stage or to loop to iterate on the stage. These votes are broadcast across all processes and evaluated by the world when determining whether or not to proceed.

```
DEFINE OPERATION
  TYPE = LogicalPoissonStripOp
  DATA_NAME = FieldData #Default
  FIELD_NAME = \phi #Default
  SOURCE_NAME = \rho #Default
  MESH_NAME = SMesh #Default
  DIRECTION = 0 #Start with X-sweep
  SUBCYCLE = 3
  DIRCYCLE = FALSE # Default TRUE
END OPERATION
```

```
DEFINE OPERATION
  TYPE = LogicalResidualOp
  FIELD_NAME = \phi #Default
  RESIDUAL_NAME = residual\_\phi #Default+(FIELD_NAME)
  SOURCE_NAME = \rho #Default
END OPERATION
```

```
DEFINE OPERATION
  TYPE = LogicalNormOp
  FIELD_NAME = \phi #Default
  RESIDUAL_NAME = residual\_\phi #Default+(FIELD_NAME)
  NORM = 2.0 #Default
END OPERATION
```

```
# Threshold Criteria to Proceed to the Next Stage
DEFINE OPERATION
  TYPE = CriteriaStageOp
  QUANTITY_NAME = SUMresidual\_\phi\_L2.00e+00
  CRITERIA = 5.0e-4 # High Density!
```
3.3. MOVE. In the next section, the particle positions are updated using the field solved in the prior step. To do this, the node centered electric field, \( E_n \), is evaluated first using the `LogicalNodeGradientOp` operator. Because the field is the negative gradient of the potential, the `FIELD_MULTIPLY_CONSTANT` of -1.0 is included. The `FIELD_GRADIENT_DIRECTIONS` are suffixes attached to the root name \( E_n \) that the operator uses to construct the three components of the field names needed to store the result.

The next two operations use the field to advance the electron and ion positions. The inputs are similar to the basic linear push described in the heatbath tutorials with extra field options so that the operator knows which field data to use for the acceleration.

After the push, the particle distribution is split between particles that remain within the domain and particles that escaped into the grounded wall. Particle that escape are marked with a `CellID` flag set within the push. This push does not actually test boundary intersections during the push which is a fast method for simple boundary conditions. Triangulated boundary surface intersecting pushes with and without field are still in testing and will appear in future revisions of the TURF-IR. The last operation in the stage is another `NextStageOp`.

```plaintext
DEFINE OPERATION
    `LogicalNodeGradientOp`
    `FieldData`
    `phi`
    `En`
    `-1.0`
    `[x, y, z]`

DEFINE OPERATION
    `SPDistESPushOp`
    `FieldData`
    `En`
    `[x, y, z]`
    `e-DST`

DEFINE OPERATION
    `SPDistESPushOp`
    `FieldData`
    `En`
    `[x, y, z]`
    `p+DST`

DEFINE OPERATION
    `SPDistSplitOp`
    `e-DST`
```
3.4. PLOT. The last stage of the simulation is plotting. The first operation in the plotting section is the CUDA accelerated real-time volume ray tracing operation, VolumeRenderOp. The code is primarily a wrapped version of the NVIDIA CUDA SDK’s VolumeRender example. The infrastructure launches that set of code in a separate window. When the operation is applied during the code’s main thread loop, a second buffer is filled from the field variable specified by the DATA_NAME and FIELD_NAME parameters. It then signals the visualization thread to swap buffers. It is restricted to single cubic domains in this version of the infrastructure because it uses the rendering kernels from the example with few modifications to apply in other geometries. Most of the settings for producing the coloring and view were obtained by interacting with the visualization to determine a ‘good’ view. This mode of interaction is described below the file listing. Other options include the commented FILE_HEAD and SAVE_IMG options. If re-enabled, the operation outputs a '.ppm' image file for every iteration that is drawn. Iteration skipping can be adjusted by the SKIP parameter to reduce the number of files. The VIEW_ORBIT parameter tells the visualization to rotate by the indicated number of degrees once per iteration automatically in addition to the interactive rotations to help make the 3D nature of the volume rendering more intuitive.
An example of the output displayed with the default settings by the realtime visualization can be seen in Figure 1. This shows the electron cloud density in the box after 828 timesteps using the default visualization parameters.
The last additional operations are a commented version of the LogicalFieldWriteVTKOp which writes the field data to output files rather than relying on the realtime visualization. This is necessary for running the tutorial on systems that do not include NVIDIA GPU’s that are compatible with the direct OpenGL interface used by the volume renderer. The options are similar to those of the heatbath tutorial. The last operation is a final NextStageOp to tell the code to advance to the next stage, or in this case, loop back to the first stage.

```
# DEFINE OPERATION
# TYPE = LogicalFieldWriteVTKOp
# DATA_NAME = FieldData
# FILE_HEAD = plt/plt_
# FIELD_NAME = Ne- CNe- Np+ CNp+ phi rho
# SKIP = 5
# # FORMAT = BINARY # Won’t open!
# HELP = TRUE
# # END OPERATION

DEFINE OPERATION
# Default Criteria to Proceed to the Next Stage
    TYPE = NextStageOp
END OPERATION

END STAGE PLOT
```

4. RESULTS

The example in this tutorial was originally developed to verify TURF functionality with respect to the ICEPIC code. Using as similar parameters as possible between the two codes, the example was run and visualized in ParaView as shown in Figure 2. The setup was nearly identical to what was outlined above except more particles were used to provide smoother output. In particular, a FILL_RATIO of 4.0 was used with the e-DST, and the default value of 0.5 was used for the p+DST to ensure a similar number of particles were used in TURF as in ICEPIC. For the realtime visualization, the low proton numbers make little difference in the electron density visualization, but they make charge density plots like those used to compare the code much more noisy. The agreement between the two codes was very reasonable considering all the particle trajectories are coupled to the field solution and vice versa. A major difference is the appearance of more charge neutrality on the surface of the ICEPIC result, but this is essentially a difference due to node-centered versus cell-centered output between the two codes. The background in ICEPIC is slightly noisier as well because the real to computational weights of particles in TURF are modified to ensure the intended cell densities rather than randomly inserting equal weight particles throughout the domain. On longer timescales after the protons have had the opportunity to move further, the noise level in TURF would appear more similar to that in the ICEPIC result. The SPDistBoxICOp available in the TURF-DEV development package would provide a more directly comparable initialization with constant particle weights, but it was added after the original verification runs were performed and will not be included in the infrastructure core until the next revision.
Fig. 2. Comparison of ICEPIC (left) and TURF (right) grounded box results
5. Appendix

Table 1. Summary of operations listed in operations.list.

<table>
<thead>
<tr>
<th>Stage</th>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>INITIAL</td>
<td>SPDistConstantIC</td>
<td>Initial particle distribution</td>
</tr>
<tr>
<td></td>
<td>SPDistCellIDDop</td>
<td>Flag cell in which particle resides</td>
</tr>
<tr>
<td></td>
<td>SPDistSortDop</td>
<td>Sort particles in cells by CellID</td>
</tr>
<tr>
<td></td>
<td>LogicalFieldSetDop</td>
<td>Set field values to constant</td>
</tr>
<tr>
<td></td>
<td>SPDistDensityToFieldDop</td>
<td>Sum real and computational particles/cell to field</td>
</tr>
<tr>
<td></td>
<td>SPDistToFieldDop</td>
<td>Sum particle charges to field entry</td>
</tr>
<tr>
<td></td>
<td>NextStageDop</td>
<td>Continue to next stage</td>
</tr>
<tr>
<td>SOLVE</td>
<td>LogicalBCConstantDop</td>
<td>Set value of cell centers in box every iteration</td>
</tr>
<tr>
<td></td>
<td>LogicalPoissonStripDop</td>
<td>Red/Black line relaxing Poisson solve</td>
</tr>
<tr>
<td></td>
<td>LogicalResidualDop</td>
<td>Calculate residual of Poisson solve</td>
</tr>
<tr>
<td></td>
<td>LogicalNormDop</td>
<td>Calculate $L^p$-norm of field variable</td>
</tr>
<tr>
<td></td>
<td>CriteriaStageDop</td>
<td>Continue to next stage if quantity below criteria</td>
</tr>
<tr>
<td>MOVE</td>
<td>LogicalNodeGradientDop</td>
<td>Calculate node-centered gradient of cell center field</td>
</tr>
<tr>
<td></td>
<td>SPDistESPushDop</td>
<td>Electrostatic particle push using node electric field</td>
</tr>
<tr>
<td></td>
<td>SPDistSplitDop</td>
<td>Split particle distribution by CellID flag</td>
</tr>
<tr>
<td>PLOT</td>
<td>VolumeRenderDop</td>
<td>Single cubic domain realtime volume rendering</td>
</tr>
<tr>
<td></td>
<td>LogicalFieldWriteVTKDop</td>
<td>Write to output files for 3D plots</td>
</tr>
</tbody>
</table>

References

TURF HEATBATH EXAMPLE - PART 1: INITIALIZATION

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CONTENTS

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1. INTRODUCTION

This tutorial is the first of two parts which give an overview of the heatbath example in TURF. Prior to running this example you should already have installed TURF and verified that it was installed properly. For information on this please read THE_INSTALL_GUIDE. All relevant files can be located in dat-SMMURF/tutorial/heatbath. You should see several files with the .list extension, which act as the scripting files for TURF. In addition to the TURF software you will also need a scientific visualization software that can read VTK files such as Paraview\(^1\) or VisIt\(^2\). Also useful is a text file comparison utility such as Meld\(^3\) or difft.

The heatbath example studies particles undergoing thermal expansion confined within a box. As mentioned before, this tutorial is the first of two parts. We will discuss setting up a coordinate system, logical domain and other necessary databases required for a TURF simulation in Section 2. It also explains the use of World-Rank.html for visualizing the simulation space. Lastly, section 3 details the addition of particles to the domain and the operations necessary for TURF to output data compatible with VisIt\(^1\). In TURF Heatbath Example: Part 2 we will discuss the details of moving particles around the domain and having these particles specularly reflect off the boundary of the domain. Lastly we will construct the same simulation using multiple domains.

\(^{1}\) www.paraview.org
\(^{2}\) https://visit.llnl.gov
\(^{3}\) http://meldmerge.org

Date: 11/25/2014.
2. world.list

Running the TURF executable in the working directory will have TURF search for the default script file, world.list, and parses it automatically. In this example, world.list is a symbolic link to the file world.heatbath.list. We can take a look at the script by opening either file.

```python
DEFINE WORLD
   NAME = Heatbath-Example
   #########################################
   ### Initially all turned off - Code does not advance ###
   ###
   ###
   #########################################
   ### Timestep advances but code does nothing ###
   ### op_file = operations.null.list ###
   #########################################
   ### Add a a particle distribution object with some ###
   ### particles in a box ###
   ### op_file = operations.addparticles.list ###
   #########################################
   ### Write vtk field output files periodically ###
   ### op_file = operations.writeoutput.list ###
   #########################################
```

We begin by defining the world and giving it a name. This name is arbitrary and can be anything. We then have a block of commented lines which are calls to different operation files. Each operation.list file when uncommented will run a different example, building on itself and adding functionality. Over the course of this tutorial we would like to elaborate on the commands used to achieve this functionality.
We then define the world coordinate system, time step, field names and stages used in the example. TURF is written to assume all units are in MKS. With this in mind, the cell size is 100µm and our time step is 1ns. The length of the simulation is defined by the \texttt{end\_time} of 250ns. Dividing \texttt{end\_time} by \texttt{start\_dt} will give us the number of iterations in the simulation, 250. Defining the various fields ensures there is memory to save the number of helium per cell and the computational number of helium per cell. The heat bath example has two stages named \texttt{INITIALIZE} and \texttt{MOVE}. A stage is a communication synchronization point after which all of the domains within the simulation can vote on whether to proceed to the next stage or repeat the current stage. This synchronization is important because different processes may finish operating on their domains before other processes do. Failure to properly synchronize may cause the simulation to produce incorrect results. Note that the names for fields and stages are only labels similarly to the world name and do not refer to any existing information in the code. However, if used elsewhere in the code it is important to reference the same name. Here we have a field named \texttt{NHe} which stores the physical number of Helium particles per cell and \texttt{CNHe} which contains the computational number of Helium particles per cell.

```plaintext
coordinates = cartesian
origin = (0.0,0.0,0.0)
delta = (100.0e-6,100.0e-6,100.0e-6)
end\_time = 250.0e-9
start\_dt = 1.0e-9

# Names Should not be fully contained in an earlier name for Plotting
fields = [NHe, CNHe]
stages = [INITIALIZE, MOVE]

END WORLD
```

Lastly we define our domain. The location of the domain is relative to the origin of the world coordinate system. The mesh spacing is global to the coordinate system and must be the same across all domains. In this example our domain is a cube with a length of 3.2mm with a mesh spacing of 0.1mm in all directions.

```plaintext
### Domain Geometry

DEFINE DOMAIN DOM000
bound\_lo = (0.0,0.0,0.0)
bound\_hi = (3.2e-3,3.2e-3,3.2e-3)

END DOMAIN
```
2.1. **operations.null.list.** The first example details the creation of a domain, followed by 250 iterations of nothing. To run this case, we uncomment the following line in the `world.list` file.

```plaintext
##########################################################
### Timestep advances but code does nothing ###
  op_file = operations.null.list ###
##########################################################
```

By doing so we call the `operations.null.list` file which defines the different operations used within the stages of the simulation. You will notice that for both the initialize stage and the move stage, there exist only one operation of the type `NextStageOp`. This operation simply tells the code to continue onto the next stage.

```plaintext
DEFINE STAGE INITIALIZE
DEFINE OPERATION
  # Default Criteria to Proceed to the Next Stage
  TYPE = NextStageOp
END OPERATION
END STAGE INITIALIZE
END STAGE MOVE
```

It is important to remember that the stage names initialize and move are just that, only names. Despite being named initialize, this stage is called every iteration and the GPU cores must sync before moving onto the move stage. As we will see in later examples, it is hard coded in the operations whether it is an initial operation or one that occurs iteratively.
When TURF is run, a html file named *World-Rank.html* is automatically generated. When opened, the user can view the object hierarchy of the example. At the base of the tree is the logical world, which was named Heatbath-Example. The branches include `GSOobject` named `GSMemberVector` which have the functionality of a vector and can be used by the GPU, there is a material database, a logical domain and the coordinate system defined by the `world.list` file. It is possible to expand the hierarchy to investigate any underlying databases or arrays which are automatically generated. Another useful feature is the visualization of the simulation environment. For this current example there exist only a single domain as shown by the blue cube. The surrounding gray region is a layer of three ghost cells which are automatically generated when the domain is formed.

![Fig. 1. World-Rank(0).html with contracted database hierarchy.](image1)

![Fig. 2. World-Rank(0).html with expanded database hierarchy.](image2)

By selecting on the visualization and pressing the ‘m’ key, we can cycle through volume view, line view and point view. This is useful for visualizing objects within the domain as we will see in the later examples.
The usefulness of the `World.Rank` output will become evident as we add functionality to example. The object hierarchy and visualization will allow us to directly see the changes we have made in the course of this tutorial.
3. Adding Particles

The following example creates a distribution of helium particles to fill a portion of the domain. We will then observe the changes made in the World.Rank file and learn how to output the data in VTK format so it can be studied using a visualization software such as VisIt.

3.1. operations.addparticles.list. To change the example we simply call a different operation.list file. We will do this by commenting out the previous op_file operations.null.list and also uncommenting the next line named operations.addparticles.list as shown below.

```
##########################################################
### Timestep advances but code does nothing ###
### op_file = operations.null.list ###
##########################################################
### Add a particle distribution object with some ###
### particles in a box ###
### op_file = operations.addparticles.list ###
##########################################################
```

If we open both operations files with meld, we can directly compare changes between these two files, we can see that there is one additional operation defined of the type SPDistConstantIC shown below. This operation does is define a box with upper and lower boundary, and distribute particles with a given number density and temperature. The particles themselves will have a given charge, mass (in units on proton mass) and drift velocity. This specific operation is an initial condition so it will only do something when it is first read.

```
DEFINE OPERATION
   TYPE = SPDistConstantIC
   DATA_NAME = He-DST
   MAX_NP = 1280000
   FILL_RATIO = 0.25
   BOUND_LO = (0.10e-3,0.10e-3,0.10e-3)
   BOUND_HI = (2.32e-3,2.32e-3,2.32e-3)
   temperature = 11604.5059 # 1ev
   number_density = 1.e14
   Z = 0
   Mass = 4.0 Mp
   vel = (0.,0.,0.)
END OPERATION
```

Since there are no push operations, the particles will remain at their locations for the length of the simulation. Looking at the World-Rank.html we can see the bounding box for which the particles will be distributed within.
Fig. 4. World-Rank(0).html visualizing both the domain and region in which particles will be distributed. You may notice the code automatically generated objects when SPDistConstantIC is called.

3.2. operations.writeoutput.list. To run the next example, open the world.list file again. Comment the line `op_file = operations.addparticles.list` and uncomment the line `op_file = operations.writeoutput.list`, similarly as before. This simulation is exactly the same as the previous except now we will output the particle density distribution in a VTK format compatible with visualization software such as VisIt. This output is generated every five iterations. To do so we will use the following operations in the move stage:

```
##############################
## Sum to Fields for Output ##
##############################
DEFINE OPERATION
  TYPE = LogicalFieldSetOp
  DATA_NAME = FieldData
  FIELD_NAME = CNHe
  VALUE = 0.0
END OPERATION
DEFINE OPERATION
  TYPE = LogicalFieldSetOp
  DATA_NAME = FieldData
  FIELD_NAME = NHe
  VALUE = 0.0
END OPERATION
DEFINE OPERATION
  TYPE = SPDistDensityToFieldOp
  FIELD_DATA_NAME = FieldData
  SPDIST_DATA_NAME = He-DST
  PSORT_NAME = Sort_He-DST
  FIELD_NAME = NHe CNHe # Computational and Physical Number per Cell
END OPERATION

######################
## Write VTK Output ##
######################
DEFINE OPERATION
  TYPE = LogicalFieldSetOp
  DATA_NAME = FieldData
  FIELD_NAME = NHe
  VALUE = 0.0
END OPERATION
```

The operation `LogicalFieldSetOp` sets the value of the field to zero for the given field name, in this case we have an operation for CNHe and another for NHe. The operation `SPDistDensityToFieldOp` sums the quantity of helium for each cell and stores it into CNHe and NHe. The last operation `LogicalFieldWriteVTKOp` outputs the field data for CNHe and NHe in VTK format every five iterations.

Opening the VTK files with visualization software such as VisIt we notice TURF has created a cube with a uniform density of helium particles just as we expected. As the simulation progresses in time, the particles remain unchanged. In the next tutorial TURF Heatbath Example: Part 2 we will discuss how to push particles through the domain and how to handle particles that leave the specified domain.

![Figure 5](image_url)

**Figure 5.** The final state of the helium particles visualized in VisIt.

### 4. Appendix

#### Table 1. Summary of operations listed in `operations.dsmc1Dshock.list`.

<table>
<thead>
<tr>
<th>Stage</th>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>INITIALIZE</td>
<td><code>SPDistConstantIC</code></td>
<td>Initial particle distribution</td>
</tr>
<tr>
<td>MOVEOP</td>
<td><code>NextStageOp</code></td>
<td>Continue to next stage</td>
</tr>
<tr>
<td></td>
<td><code>SPDistDensityToFieldOp</code></td>
<td>Sum particles per cell for field entry</td>
</tr>
<tr>
<td></td>
<td><code>SPDistSortOp</code></td>
<td>Sort particles according to cell ID</td>
</tr>
<tr>
<td>POSTOP</td>
<td><code>LogicalFieldSetOp</code></td>
<td>Initialize the field parameters</td>
</tr>
<tr>
<td></td>
<td><code>LogicalFieldWriteVTKOp</code></td>
<td>Write to output files for 3D plots</td>
</tr>
</tbody>
</table>

#### References

1. Introduction

This tutorial is the second of two parts which give an overview of the heatbath example in TURF. If you have not yet gone over the first heatbath tutorial, it is advised that be done prior to running this example. You should already have installed TURF and verified that it was installed properly. For information on this please read THE_INSTALL_GUIDE. All relevant files can be located in dat-SMMURF/tutorial/heatbath. You should see several files with the .list extension, which act as the scripting files for TURF. In addition to the TURF software you will also need scientific visualization software that can read VTK files such as Paraview\(^1\) or VisIt\(^2\). Also useful is a text file comparison utility such as Meld\(^3\) or diff.

In the first part of the heatbath tutorial we discussed the basics of constructing a world coordinate system, domain and the operations needed to add particles to the simulation. In this tutorial we plan on expanding our simulation by adding a time dependence. Section 2 we will discuss how to thermally expand particles and how to handle particles which have left the domain. In Section 3 we will impose boundary conditions which specularly reflect incoming particles, thus completing the heatbath example. Lastly, we would like to construct the same simulation with multiple domains requiring changes to both the world.list and operations.list files.

\(^1\)www.paraview.org
\(^2\)https://visit.llnl.gov
\(^3\)http://meldmerge.org
2. Particle Pushing

In TURF Heatbath Example: Part 1 our final example had particles which remained stationary for the length of the simulation. The next logical step is to allow the particles to thermally expand.

2.1. operations.push-untrimmed.list. Pushing particles is quite simple, requiring one additional operation. We begin by running the operations.push-untrimmed.list file the same way as before. In this case after initially distributing the particles in a cube, the operation SPDistMoveOp will thermally expand the particle distribution over time.

```plaintext
DEFINE OPERATION
  TYPE = SPDistMoveOp
  SPDIST_DATA_NAME = He-DST
END OPERATION
```

You may notice the total number of particles in the simulation decreasing over time. This is due to a lack of boundary conditions for our domain; particles continue on their trajectory beyond the bounds of the simulation.

![Fig. 1. The final state of the helium particles visualized in VisIt for the push-untrimmed example.](image)

2.2. operations.push.list. Running this example shows an output identical to the push-untrimmed case however, it now has functionality to sort through the particle list and explicitly remove those that have moved into the ghost cells as opposed to the previous example where these particles would be ignored and continue on their trajectory. It does so using the following operations:
From the previous example we have added a distribution for helium named He-GST. The operation `SPDistCellIDOp` determines what cell every particle is in and the operation `SPDistSortOp` moves particles in ghost cells from He-DST to He-GST.

**Fig. 2.** The final state of the helium particles visualized in VisIt for the push example.
3. Particle Heatbath

3.1. operations.heatbath.list. The final example is the particle heatbath, thermally expanding in a box. To do so, we impose boundary conditions and have particles specularly reflect off the walls of the domain. By running operations.heatbath.list, we use an operation named SPDistBCSpecOp which creates a region that share a surface with the domain. These regions will reflect incoming particles in a given direction. An example of the use of this operation is shown below. The code requires us to write this operation six times, one for every surface of the cubic domain. A visualization of these regions can be seen below in the .html file.

```plaintext
### 1-Walls reflect particles ###

DEFINE OPERATION
    TYPE = SPDistBCSpecOp
    DATA_NAME = He-DST
    DIRECTION = xm
    BOUND_LO = (-100.e-4,-100.e-4,-100.e-4)
    BOUND_HI = ( 0.00001e-4, 132.e-4, 132.e-4)
END OPERATION
```

Fig. 3. World-Rank(0).html visualizing both the domain and boundary condition region which specularly reflects incoming particles.

Taking a look at the output in VisIt we notice the total number of particles remains unchanged. If the simulation is run longer, it will eventually approach steady state.
3.2. Multiple Domain Case. The final example demonstrates the ability to use multiple domains. Doing this requires us to change the domain geometry in the world.list file. Luckily for us we already have a file we can change the pointer to named world.heatbathx2.list. We first remove the previous pointer and create a new pointer with the same name to world.heatbathx2.list.

```
user@comp:/SMMURF$ projects/dat-SMMURF/> rm world.list
user@comp:/SMMURF$ projects/dat-SMMURF/> ln -s world.heatbathx2.list world.list
```

Comparing the two world.list files the domain geometry is the only modification.

```
DEFINE DOMAIN DOM000
  bound_lo = (0.0,0.0,0.0)
  bound_hi = (1.6e-3,3.2e-3,3.2e-3)
END DOMAIN

DEFINE DOMAIN DOM001
  bound_lo = (1.6e-3,0.0,0.0)
  bound_hi = (3.2e-3,3.2e-3,3.2e-3)
END DOMAIN
```

When using multiple domains, it must be possible to exchange particles between the different domains. Looking at the operations.list file we notice two significant differences between the single domain and multiple domain cases. The first of which handles the exchange of particles from one domain to the other using a distribution named He-EXC. The operation `SPDistCombineOp` unifies the particles from He-EXC distribution with He-DST at the beginning of every loop.

```
DEFINE OPERATION
  TYPE = SPDistConstantIC
  DATA_NAME = He-EXC
  MAX_NP = 1280
```

Fig. 4. The final state of the helium particles visualized in VisIt for the heatbath example.
END OPERATION

############################################
## Combine EXC into DST from Patch at End of Move Stage ##
############################################
DEFINE OPERATION
    TYPE = SPDistCombineOp
    SRC_DATA_NAME = He-EXC
    DST_DATA_NAME = He-DST
# VERBOSE = TRUE
END OPERATION

If the particle moves between the two domains, it is temporarily removed from He-DST placed into the distribution He-EXC until the beginning of the next iteration which we saw in the previous block of code.

############################################
## Split Particles Still Outside Active Domain for Patch ##
############################################
DEFINE OPERATION
    TYPE = SPDistCellIDOp
    DATA_NAME = He-DST
END OPERATION
DEFINE OPERATION
    TYPE = SPDistSplitOp
    SRC_NAME = He-DST
    DST_NAME = He-EXC
END OPERATION
DEFINE OPERATION
    TYPE = SPDistPatchOp
    SRC_NAME = He-EXC
    DST_NAME = He-EXC
END OPERATION
DEFINE OPERATION
    TYPE = NextStageOp
END OPERATION

Running the simulation we see that the output is similar to the single domain heatbath case as we would expect it to be, do note however in the world.list file the overlapping ghost cells in the volume domain which are required for the exchange of particles between domains.
Fig. 5. Volume domain split into two pieces.

Fig. 6.

This completes the TURF Heatbath Example. If you have any questions or concerns, please direct them to Jonathan Tran\(^4\) at ARFL/RQRS.

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4. Appendix

Table 1. Summary of operations listed in operations.dsmc1Dshock.list.

<table>
<thead>
<tr>
<th>Stage</th>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>INITIALIZE</td>
<td>SPDistConstantIC</td>
<td>Initial particle distribution</td>
</tr>
<tr>
<td>MOVEOP</td>
<td>NextStageOp</td>
<td>Continue to next stage</td>
</tr>
<tr>
<td></td>
<td>SPDistMoveOp</td>
<td>Advancement of particles</td>
</tr>
<tr>
<td></td>
<td>SPDistDensityToFieldOp</td>
<td>Sum particles per cell for field entry</td>
</tr>
<tr>
<td></td>
<td>SPDistSortOp</td>
<td>Sort particles according to cell ID</td>
</tr>
<tr>
<td></td>
<td>LogicalFieldSetOp</td>
<td>Initialize the field parameters</td>
</tr>
<tr>
<td></td>
<td>SPDistBCSpecOp</td>
<td>Specularly reflecting boundary condition</td>
</tr>
<tr>
<td></td>
<td>SPDistCombineOp</td>
<td>Unifies the particles from different distributions</td>
</tr>
<tr>
<td></td>
<td>SPDistCellIDOp</td>
<td>Marks the cell ID in which particles reside</td>
</tr>
<tr>
<td></td>
<td>SPDistSplitOp</td>
<td>Splits particle distribution into two by cell ID</td>
</tr>
<tr>
<td></td>
<td>SPDistPatchOp</td>
<td>Transfers particles between domains</td>
</tr>
<tr>
<td>POSTOP</td>
<td>LogicalFieldWriteVTKOp</td>
<td>Write to output files for 3D plots</td>
</tr>
</tbody>
</table>

References