Particles Breakout Session

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The session was initialised by James Cook (JC) describing NEPTUNE requirements for a particle framework. Such a framework should be capable of more complex interactions such as charge-charge, charge-neutral and particle-wall whilst describing important physical processes. Peter Coveney (PC) described additional uses of particle (plus Finite Element Method (FEM)) techniques that were of interest to many people. This broad set of use cases and general use of the word "particle" raises the point that "particle" covers a wide range of applications. Particles can be points, blobs, atoms, species etc whilst representing many length scales, e.g. atoms vs mesoscopic quantities. Different NEPTUNE grantees have different use cases for particles that span a range of length/time scales and computational complexity.

JC introduced to that in the NEPTUNE use case we envisage a hybrid representation to be appropriate for species that exist in both collisional and collision-less regimes. The burning plasma can be suitably considered as a collision-less environment where a kinetic representation is required and that particles are a suitable kinetic representation. This kinetic representation would exist over a so called 3+3 phase space of 3 positional dimensions and 3 momentum dimensions. The latter momentum portion of the phase space is representable with a particle distribution. However, one of the drawbacks of particle representations is that, without careful attention, they can be accompanied by a significant noise contribution. Noise can be reduced by increasing the number of particles to sufficiently resolve the relevant physics. It was pointed out that the number of simulated particles will be many orders of magnitudes less than the actual numbers of atoms in the plasma.

JC covered the NEPTUNE use case where particles are both charged and neutral and both species are required to model non-trivial cases such as detached plasma. These interesting cases also require inter-particle interactions to represent the collisional interactions between species. As the number of species increases the number of inter-species collision operators increases accordingly and the particle framework should allow the physically relevant subset of these operators to be described. It may be desirable to convert particle representations to fluid representations in sufficiently collisional regimes, and vice versa, based on prior knowledge or runtime calculated metrics. This promotes an implementation and framework that supports a hybrid representation through the mathematical model and libraries such as coupling frameworks.

PC points out that JC is confirming that that "particles" has a wide range of meanings and represents different length/time scales in different contexts. JC describes that a simulation may have 1E9-1E12 particles that each represent many real-world particles. In certain circumstances there may be a one to one correspondence between simulation particles and real-world particles. Martin O'Mullane (MOM) points out that molecules are also involved and are of interest.

A more complex example could split and recombine these molecules. JC confirms that we do need to handle molecules.

Steven Wright (SW) states that PIC codes are usually implemented in a collisionless manner and asks how we will develop a collisional implementation. JC suggests that we start with particle-background collisions against a fixed background quantity. Robert Kingham (RK) points out that species exist in different states, e.g. electron states. MOM states that the physics of the molecules in the plasma may significantly vary based on the temperature of the plasma and that this can involve quite complex processes due to the significant number of possible states. JC points out that the implementation of these processes would require the operators and rates to be know and implemented. MOM suggests a model reduction approach to extract the key processes and hence reduce the complexity/required information. MOM also remarks that some processes will be rare and some processes will reverse on very small time scales. Rob Akers (RA) suggests that surrogate models can be made for these complex processes and that the MetOffice has surrogate models for physical processes. A discussion over continuum/diffusion models occurs with reference to existing work studying chemical processes. Care needs to be taken when producing these models due to the underlying complexity and stiffness of the equations.

RA inquires what resource/effort should be applied to appropriately move forward with these models of physical processes. MOM suggests that effort and users are required but it is currently unclear how to apply a molecular population model to NESO. JC points out that SYCL code for operations can be generated, i.e. from a know set of functional forms and provided coefficients NESO can potentially generate much of the boilerplate code. MOM suggests this would be nice to do as a collaboration to which RA asks what would make good starting project. MOM suggests a hydrogen population model that coupled to NESO, RA points out that we will in future want molecules in NESO.

A general discussion follows over the effect of techniques that avoid loosing particles on the final solution, i.e. does these techniques induce artificial diffusion into the simulation and is this at a significant magnitude. These discussions touch on topics such as particles passing through vertices and gyrating particles.

MOM introduces a discussion point covering the wide, and potentially sharp, temperature profiles that should be resolved in a simulation. JC suggests we exploit the functionality in Nektar++ that exists to capture boundary layer flows in CFD simulations to provide resolution where needed for our use case. RA asks if we consider an Adaptive Mesh Refinement (AMR) scenario - JC indicates that we do not exclude AMR. MOM posits that the simulation will start in a "nice" regime and evolve into a regime with more complex structures that are to be captured and that it is not known a prior where to do the refinement. This discussion evolves to cover processes such as ELMS. JC points out that we are building the ground work now then can evolve to cover these more complex cases, i.e. a framework of components to build complex implementations. Nice-to-haves would include a Finite Element Exterior Calculus (FEEC) capability.

RA asks what we think our involvement with Exascale RSE should look like - general consensus is that we should definitely be involved from an early stage. JC points out that we are developing connections with relevant people in the SYCL community. A general discussion over the direction of SYCL follows. Will Saunders (WS) points out that we also have a significant interest in describing and scheduling tasks.

A relatively short and broad discussion follows touching on topics such as gyrokinetics, hybrid representations, the possibility of dust modelling and the inclusion of fuel pellets. The fuel pellets are interesting/challenging as they are a high-gradient object in the simulation that may require techniques such as h and p refinement to represent. The final short discussion promotes collaboration between NEPTUNE and FARSCAPE.