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In photo: The world map from the 1572 *Theatrum Orbis Terrarum* by Abraham Ortelius, first complete atlas of the world. Public domain image from Wikipedia.

Redrawing the map: new Grand Challenges for SPH

Angelantonio Tafuni

In 2027, Smoothed Particle Hydrodynamics will mark fifty years since Lucy, Gingold and Monaghan introduced it as a tool for astrophysics. Half a century later, SPH is used to design ships, aircraft and medical devices, forecast floods and lava flows, study magnetohydrodynamics, and much more. It is a fitting moment to ask what still stands between the method and its full maturity.

SPHERIC first posed this question 12 years ago through its Grand Challenges, reviewed in Issue 27 of this newsletter. Much has changed since. Boundary conditions, variable resolution and coupling with mesh-based solvers have matured considerably, while computing hardware has become massively parallel and heterogeneous, machine learning has entered computational mechanics, and SPH is now applied to problems in which several physical processes interact. The SPHERIC Steering Committee has therefore revised the list. This issue presents five new Grand Challenges, spanning from the foundations of the method to its use: Mathematical and Numerical Foundations (GC1), Advanced Physical and Multi-Physics Modeling (GC2), Efficient and Intelligent Algorithms (GC3), High-Performance and Heterogeneous Computing (GC4), and Scientific and Engineering Applications (GC5).

Although written independently, the contributions share common threads. All of them call for verifiability, whether through criteria for conservation and entropy production, separation of physical and numerical dissipation, or transparent validation. Several stress the balance between accuracy and computational cost, and the need for shared benchmarks and data on which methods can be compared. Above all, the challenges are interdependent. An adaptive scheme that breaks conservation, a multiphysics model that cannot run at scale, or an efficient algorithm that cannot be ported to modern hardware does not advance the method as a whole.

The new list will replace the former one on the SPHERIC website. Like its predecessor, it is intended as a living document, and we invite the community to suggest references, identify gaps and contribute to this collective effort.

Grand Challenge 1 (GC1): Mathematical and Numerical Foundations

Chun Hean Lee, Abbas Khayyer

SPH has developed from a relatively simple particle discretisation into a broad family of methods for increasingly complex problems in fluid, solid and multi-physics mechanics. Its flexibility is a major strength, particularly for large deformation, fragmentation, free surfaces, moving interfaces and changing topology. At the same time, the diversity of SPH formulations, correction procedures, stabilisation techniques and multi-physics extensions has made it difficult to establish a common understanding of their mathematical and numerical properties. The new GC1 aims to strengthen these foundations by providing a direction for the development and assessment of SPH methods. The objective is not to identify a single preferred SPH formulation, but to establish principles that allow different approaches to be analysed, compared and systematically improved. The central challenge is to maintain a connection between the continuum equations and their discrete particle representation, including the effects of stabilisation, correction, particle motion, boundaries and coupling. This requires a consistent treatment of conservation, consistency, stability, convergence and thermodynamics throughout the formulation.

Variational and discrete consistency. Many SPH formulations can be derived from a discrete variational principle [1], providing a systematic basis for conservation of linear and angular momentum. In practice, however, additional terms are often introduced to control particle disorder, tensile instability [2,3] or spurious numerical oscillations. These modifications can change the underlying discrete structure. A fundamental challenge is therefore to establish the mathematical role of such corrections and stabilisation terms. Their effects on the variational structure, conservation and consistency should be understood at the discrete level rather than assessed only through numerical robustness. This is particularly important because corrections that improve field reproduction may affect exact conservation, whilst conservative formulations may suffer from consistency errors for irregular particle distributions or near boundaries. Developing a framework to understand these trade-offs is central to the mathematical foundation of SPH.

Thermodynamic consistency and dissipation. Thermodynamic consistency [4] is equally important, particularly for dissipative and multi-physics problems. The discrete formulation should have a clear relationship with the first and second laws of thermodynamics, and numerical dissipation should be controlled rather than introduced solely to suppress numerical oscillations. This applies to artificial viscosity, Riemann-solver-based dissipation, particle shifting, stress corrections [5] and other stabilisation mechanisms. Their effects on energy and entropy production need to be established at the discrete or semi-discrete level. In particular, the use of a Riemann solver does not by itself guarantee thermodynamic consistency; the complete discretisation, including reconstruction, limiting, flux evaluation and time integration, determines the resulting properties. GC1 should therefore establish general criteria for energy conservation, controlled dissipation and non-negative entropy production to guide the development and assessment of SPH schemes.

Consistency, patch tests and stability. A fundamental challenge is to establish if the discrete SPH equations reproduce basic continuum states. For example, under a constant stress state and in the absence of external forces, the discrete internal force should vanish, giving zero acceleration and preserving equilibrium. Patch tests therefore provide a simple and fundamental measure of discrete consistency and should be considered for both regular and irregular particle distributions. This requirement must be considered along with numerical stability. Zero-energy modes, rank deficiency, tensile instability and other numerical instabilities can persist even when basic consistency requirements are satisfied, whilst stabilisation may suppress these modes at the expense of other properties. Particle shifting, adaptive resolution and variable smoothing lengths can further modify the discrete equations and therefore require analysis of their effects on consistency, conservation and stability. Convergence studies should quantify how particle resolution, smoothing length, particle disorder and stabilisation affect discretisation errors and convergence rates, with manufactured solutions providing controlled tests where analytical solutions are available. For example, a manufactured torsional deformation problem has been proposed, with details provided in the SPHERIC Benchmark Test 24 [6]. Boundary treatment forms part of the same mathematical problem. Kernel truncation near boundaries can introduce consistency and conservation errors, whilst boundary corrections may themselves introduce spurious forces or energy that are not present in the continuum problem. Boundary treatments should therefore be analysed within the same mathematical framework as the interior discretisation, so that their effects on consistency, conservation and stability can be measured and controlled.

Multiphysics and interface coupling. The increasing application of SPH to multi-physics problems (discussed in more detail in Grand Challenge 2) introduces a further foundational challenge. Combining models that are individually consistent does not automatically guarantee that the complete discrete system satisfies the required conservation and thermodynamic properties. Coupling terms should therefore be derived and

assessed in relation to the mass, momentum and energy balances and, where appropriate, entropy production. This is relevant to FSI [7], multiphase and thermo-mechanical problems [8], as well as coupling between SPH and other numerical methods such as FEM/FVM and other discretisation techniques. A key challenge is to formulate coupling and interface conditions that ensure consistent transfer of momentum and energy between the coupled systems, without introducing spurious forces, energy imbalance or other interface artefacts.

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Grand Challenge 2 (GC2): Advanced Physical and Multi-Physics Modeling

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Evolution of SPH from single-physics to multi-physics models

Although its origins in astrophysics can be argued as addressing multi-physics problems, over the past few decades, Smoothed Particle Hydrodynamics (SPH) has mainly evolved as a solver for single-physics flow problems. Despite this, the SPH method also provides formulations for turbulence, capillarity and wetting, heat transfer and phase change, fluid-structure interaction (FSI), fracture and fragmentation, and magnetohydrodynamics (MHD) [1–5]. The central challenge is therefore no longer simply whether an individual physical process can be represented in SPH, but whether multiple physical descriptions can interact without compromising the accuracy, conservation properties, stability, and range of applicability of their constituent models. This distinction is particularly important because physical evolution and particle discretisation are often mutually dependent. Turbulence modelling may require modified particle transport or regularisation; evaporation can produce particle-mass disparities that motivate adaptivity (splitting or merging of particles); cavitation generates large density and particle-volume changes; and fracture removes neighbours and alters the support through which the continuum is approximated. The particle representation is therefore not merely a passive discretisation of the coupled physics. In many multiphysics problems, it evolves as part of the physical–numerical system and feeds back into the predicted solution. We therefore define the grand challenge of advanced physical and multiphysics modelling as the development of SPH frameworks in which four requirements are satisfied simultaneously: (i) exchanges of mass, momentum, energy, and problem-specific quantities remain physically and discretely consistent; (ii) evolving particle representations remain compatible with the coupled physical models; (iii) physical modelling scales and numerical resolution remain compatible in space and time; and (iv) physical transport and dissipation can be distinguished from numerical regularisation and stabilisation. These requirements must also be verifiable, such that errors arising from physical closure, discretisation, coupling, and stabilisation can be separately diagnosed.

Four types of applications with multiphysics coupling challenges

Transport and closure coupling: turbulence. Turbulence is among the first physical processes to expose the difficulties of multiphysics coupling in SPH. It demonstrates that introducing a closure model is insufficient unless the closure remains compatible with particle transport, pressure evaluation, resolution, and numerical dissipation. Particle rearrangement induced by background pressure can contaminate the high-wavenumber energy spectrum, illustrating that regularisation may influence the same scales represented by the turbulence model. Similar issues arise in wall-bounded, multiphase, and complex-boundary flows. Extending turbulence modelling to deforming interfaces therefore requires control of both the physical closure and the dissipation introduced to maintain particle regularity.

Interface and state-transition coupling: capillarity, wetting, heat transfer and phase change. Capillarity and wetting require consistency among interface geometry, surface-tension forces and interfacial energy. Although continuum surface force and pairwise-force models reproduce many interfacial behaviours, moving contact lines and dynamic contact angles remain challenging, particularly when physical dissipation and numerical stabilisation interact.

Heat transfer and phase change introduce latent heat and interfacial mass exchange, potentially modifying particle mass, volume and resolution. Thermo-capillary melt-pool models couple melting, wetting, Marangoni stresses and recoil pressure, but resolving ambient gas does not necessarily resolve vapour transport or evaporation mass fluxes. The distinction between resolved physics and constitutive closures should remain explicit.

Cavitation adds rapid pressure-driven state changes and large density variations. An equation of state alone may not capture non-equilibrium mass transfer. Predictive cavity dynamics and collapse loads require consistency between phase-change closure, adaptive particle resolution, turbulent transport and numerical regularisation.

Topology-changing coupling: fracture and fragmentation. Fracture directly changes the particle support on which SPH relies. Damage-based and total Lagrangian formulations model fragmentation and crack propagation, while phase-field and nonlocal approaches seek to regularise crack evolution and address support deficiency. Assessment must therefore consider fracture energy, load response, and crack paths while incorporating dynamic refinement of the discretisation rather than only the ability to produce fragmentation.

Coupling of SPH with the Finite Element Method (FEM) or peridynamics (PD) provides alternative routes for modelling, and such approaches extend SPH towards fluid–solid–failure modelling but even so questions remain concerning interface accuracy, conservation between particles of different sizes, and the subsequent transport of generated debris. A main challenge is then to develop algorithms for treating fracture and fragmentation, and develop structural elements

such that coupling of the SPH method to other methods is not required.

Constraint-preserving coupling: magnetohydrodynamics. MHD requires SPH to evolve the fluid and magnetic fields while controlling the divergence-free constraint. Conservative SPMHD formulations provide compatible magnetic-field evolution, momentum, energy, shock capturing, and variable smoothing lengths [6,7]. However, tensile-instability corrections may compromise exact momentum conservation, while magnetic pair forces do not generally conserve angular momentum exactly. Additionally, no generally robust method for exact divergence preservation has yet been established [5]. Non-ideal effects introduce further coupling e.g. Ohmic resistivity, ambipolar diffusion, the Hall effect. Artificial resistivity adds resolution-dependent diffusion. MHD coupling consequently requires consistent energy exchange, constraint control, and separate assessment of physical and numerical dissipation.

Requirements for multiphysics coupling

Across these problems, four recurring requirements determine whether multiphysics SPH is genuinely coupled rather than assembled from independently successful modules.

Exchange consistency. Coupled models exchange mass, momentum, and energy and may additionally exchange latent heat, interfacial work, fracture energy, or magnetic energy. The discrete exchange should reproduce the intended physical balance without introducing unaccounted numerical sources or sinks.

Compatibility of the particle representation. Changes in particle mass, volume, smoothing length, neighbourhood, or connectivity modify consistency, resolution, and numerical dissipation. Physical closure and particle representation therefore cannot always be designed independently, particularly when the physics drives particle redistribution, volume adaptation, splitting and merging, or support loss.

Compatibility of physical and numerical scales. Refinement may change not only discretisation error but also physically relevant modelling scales, including the LES filter length, fracture regularisation length, interface thickness, curvature resolution, and multi-resolution coupling length. Acoustic, viscous, capillary, thermal, chemical, magnetic, and mechanical processes may likewise evolve on very different time scales, which requires careful construction of time-integration schemes.

Separation of physical and numerical dissipation. Artificial viscosity, particle shifting, background pressure, tensile-instability corrections, and artificial resistivity may be essential for a viable discretisation, but their effects must not be confused with physical transport. The relevant question is not only whether a coupled calculation remains stable, but whether physical dissipation remains identifiable when numerical regularisation acts simultaneously. A robust verification process is essential.

Outlook

The next advance in multiphysics SPH will not be measured by the number of physical modules that can be added, but by whether their interactions remain physically consistent, discretely compatible, and systematically verifiable as the particle representation evolves. The priority is to develop coupling frameworks in which exchange balances, scale interactions, numerical regularisation, and topology changes can be diagnosed and controlled. Data-driven discretisations provide a possible route towards adaptive closure and transport modelling in SPH [8]. Their extension to multiphysics problems should, however, be judged by the same requirements of conservation, scale compatibility, dissipation control, and verifiability as physics-based formulations. Achieving these capabilities would move SPH from the simulation of increasingly complex processes towards predictive multiphysics modelling with attributable uncertainty and error. In this sense, multiphysics coupling is not an optional extension of SPH, but the central test of its development into a general-purpose modelling framework.

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Grand Challenge 3 (GC3): Efficient and Intelligent Algorithms

Angelantonio Tafuni, Guillaume Oger

SPH operators are evaluated through kernel-weighted interactions over the support of each particle, which requires repeated neighbour searches and many pairwise evaluations. Because accuracy is tied to particle spacing and kernel size, increasing resolution rapidly inflates the number of degrees of freedom, particularly in three dimensions. As a result, SPH is often reserved for problems that no other method can address, rather than chosen on merit for those that several can. GC3 concerns methods that improve solution fidelity for a given computational cost: adaptive resolution, hybrid and coupled formulations, reduced-order modelling and AI-driven approaches. The first two extend earlier Grand Challenges on adaptivity and coupling, while the latter two are emerging fields whose role in SPH now warrants explicit consideration.

Adaptive and variable resolution. Variable resolution has evolved from a research demonstration into a working capability of several SPH codes. Particle-level refinement, by splitting and merging or within overlapping regions guided by coarse parent particles, now operates in three dimensions with large refinement ratios and extends to compressible multiphase flows [1]. Dynamic splitting and merging with direct interactions between refinement levels offers very local refinement and a wide choice of refinement criteria. These interactions nevertheless raise open questions on particle distributions and the need for particle shifting, on the treatment of particle neighbourhoods, and on the accuracy of conservative versus non-conservative formulations, particularly near a free surface [2]. A complementary route assigns fixed resolutions to different materials or zones, coupled through interfaces, as in multi-resolution fluid-structure interaction [3] and domain decomposition [4] (Fig. 1). Since the smallest particles dictate the global time step, multiple and local time stepping [3,5] is needed to turn multi-resolution into a multi-scale capability. Three questions define the challenge: how refinement can be driven by an estimate of the discretization error rather than by geometric or feature-based criteria, how conservation and consistency can be guaranteed across resolution interfaces within the framework of GC1, and how free surfaces and material interfaces can cross resolution boundaries without problem-specific treatment. In addition, such algorithms must remain portable and efficient on massively parallel CPU and GPU architectures.

Hybrid methods and coupled schemes. SPH can be used efficiently by restricting it to the regions where its Lagrangian, meshless character is advantageous and treating the remainder with finite-volume or finite-element solvers, potential-flow or depth-averaged wave models, or structural and discrete-element formulations. Such couplings, typically based on domain decomposition as in SPH-finite volume coupling [6] or on partitioned SPH-FE approaches, can deliver results beyond the reach of pure SPH. Like variable resolution, they require mass, momentum and energy to be exchanged consistently between discretizations that share neither nodes nor time steps, and buffer techniques developed for open boundaries offer a natural framework for this exchange. Open questions include the stability of partitioned schemes when the subsystems differ strongly in stiffness or time scale, added-mass effects at low structure-to-fluid density ratios, and error control in mixed-fidelity simulations, where the contribution of each subsystem to the global accuracy is generally unknown.

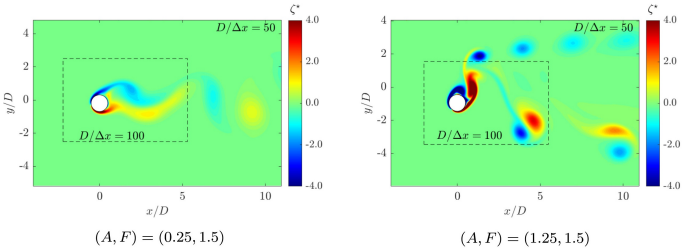


Fig. 1: Dimensionless vorticity contours from SPH simulations of flow past an oscillating cylinder obtained with a moving domain-decomposition approach developed in [4].

Reduced-order models. Design optimization, uncertainty quantification, control and digital twinning require hundreds to thousands of evaluations of a parameterized system, which is out of reach at the cost of a full SPH simulation per evaluation. Reduced-order models replace the particle system with a low-dimensional representation, built either non-intrusively from the system response or intrusively by projection of the governing equations. In the non-intrusive setting, Martinez-Carrascal *et al.* [7] used δ-SPH simulations to calibrate bouncing-ball models of violent vertical sloshing across liquid properties and filling levels, reproducing dissipation and sloshing forces at negligible cost, although such models predict integral quantities rather than the flow field. Intrusive reduction has been hindered in SPH by a structural difficulty: snapshot-based modal decomposition presumes a fixed correspondence between degrees of freedom and spatial locations, whereas particles advect, mix, enter and leave the domain. Proper orthogonal decomposition has been applied directly to particle fields where mixing is limited [8], and Rodriguez *et al.* [9] addressed the difficulty at its root through modal reference spaces, in which snapshots are decomposed before the reduced representation is returned to the particles by scattered-data interpolation, so that the SPH equations can be evolved by Galerkin or Adjoint Petrov-Galerkin projection. As the

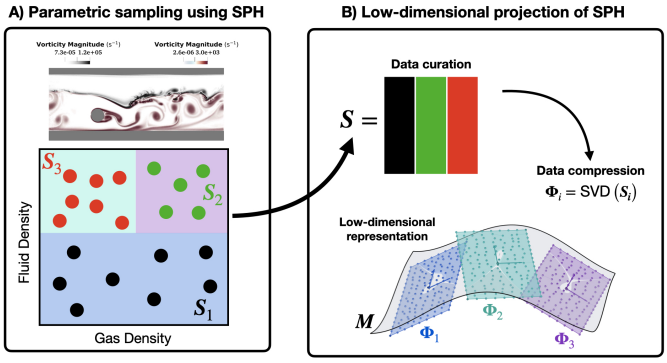


Fig. 2: Projection-based reduced order modelling using SPH. A) Two-dimensional parametric sampling of multiphase flow using SPH. B) Low-dimensional projection of SPH requires careful data curation of a meshless data structure onto a reference space, which can then be compressed into affine bases that represent different areas of the solution manifold $\mathcal{M}$.

authors note, computational savings still require hyper-reduction strategies compatible with a continuously mixing topology, and the pressure field remains sensitive to acoustic content inherent to the weakly compressible formulation, a manifestation of the dissipation issues discussed in GC1. The challenge therefore comprises meshless hyper-reduction, subspace construction robust to high-frequency content, extension to free-surface and topology-changing flows, and parametric generalization with rigorous error estimates (Fig. 2).

Data-driven and AI-assisted SPH. Machine learning has entered particle methods along a spectrum defined by how much of the SPH solver is retained. End-to-end learned simulators, in which a graph neural network predicts particle behavior from the local neighbourhood, are fast at inference but drift over long rollouts and extrapolate poorly. The LagrangeBench suite [10] provided SPH-generated benchmarks for systematic comparison, and subsequent work showed that reintroducing SPH ingredients into learned simulators substantially improves rollout stability [11], while for turbulence, generalization was found to improve as more SPH structure is enforced [12]. Hybrid formulations, in which the solver is retained and only selected terms are learned, therefore appear most promising for engineering use. Huo *et al.* [13] followed this route for microgravity sloshing, learning surface tension as the gradient of a surface energy so that momentum is conserved by construction, and recasting the solver as sparse graph operations that share a single GPU framework with the network. Differentiable SPH implementations [14] make such embedded training systematic and enable gradient-based calibration, inverse problems and shape optimization with SPH in the loop. Recurring open questions are how conservation and consistency can be built into learned components rather than expected to emerge from training, how learned models can be validated beyond their training conditions, and how methods can be compared when each group relies on its own data.

GC3 asks of the community. 1) *A SPHERIC dataset for reduced-order and learned models*, built from the existing validation benchmarks, so that training data, test data and reference solutions are shared. 2) *Reporting accuracy against cost*. Efficiency claims for adaptive, coupled, reduced or learned methods are hard to verify when speed-ups are quoted against different baselines, often a non-optimized version of the same code. Reporting error and cost against a uniform-resolution SPH reference on a shared benchmark would make progress on GC3 measurable.

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Grand Challenge 4 (GC4): High Performance and Heterogeneous Computing

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With progress being made against the Grand Challenges in SPH, the necessity for faster and more efficient simulations is inexorably increasing. With the comparatively large stencils of particles and unstructured nodal connectivity, data structures and memory layouts become challenging, while the requirements for resolved simulations demand the use of acceleration via hardware on a large scale. This is further complicated by the rapid evolution of hardware which is increasingly diverse and heterogeneous as exemplified by many of the world's top supercomputers.

This then entails multiple challenges including (but not limited to):

- Scalable parallel algorithms
- Multi-accelerator systems
- Distributed heterogeneous architectures
- Memory and I/O optimisation
- Code portability
- Energy-efficient execution

In this future, there is an opportunity to develop scalable algorithms on heterogeneous architectures which are well suited to the *n*-body type algorithms and Lagrangian particle methods such as SPH. The target is not only the scalability on distributed architectures but also portability, and algorithms which are energy efficient.

Brief hardware and software background

Originating in astrophysics in 1977, SPH subsequently adopted distributed-memory message passing, CPU vectorisation and shared-memory parallelism. Co-processors and GPU computing accelerated engineering codes such as DualSPHysics [1], GPUSPH [5] and SPHinXsys [11], while large astrophysical codes developed complementary approaches: e.g. GADGET-4 [3] combined MPI with shared-memory communication, SWIFT [12] used fine-grained tasks and asynchronous communications and lately SPH-EXA [4,9] combined distributed decomposition with GPU execution [1–5,9]. These developments established that SPH can exploit large parallel systems, but hardware diversity now makes data movement, scheduling and software sustainability central concerns. Emerging exascale and AI-oriented systems combine many-core accelerators, tightly coupled CPU–GPU nodes and deeper memory hierarchies under power constraints [6,8,10].

Emerging parallel architectures

Scalable parallel algorithms must accommodate particles with variable smoothing lengths, different neighbour counts and uneven multiphysics costs. Equal particle counts therefore need not imply equal work. Future decomposition should use measured interaction and timestep costs, balance work dynamically, and limit particle migration and halo volume. Task graphs offer a way to overlap independent work and communication, as explored in SWIFT [2,12] and SPH-EXA's demonstrated distributed GPU-capable octree construction [4]. The challenge is to reduce synchronisation without violating numerical dependencies. Strong and weak scaling should be assessed on adaptive, non-uniform workloads over complete simulations.

Multi-GPU systems increase both throughput and aggregate memory, and solvers such as GPUSPH and DualSPHysics already support multiple GPUs [1,5]. Future implementations may partition work topology, advance halo communications, and overlap boundary transfers with interior interactions. As strong scaling reduces the work per GPU, communication, neighbour-search and global reductions can dominate. Maintaining enough concurrent work becomes particularly difficult in such algorithms. There is an opportunity to coordinate spatial decomposition, timestep scheduling and GPU batching, rather than optimise interaction kernels in isolation.

The PKDGRAV3 code takes a similar and complementary approach [14]. Designed for planetary-scale impact simulations, PKDGRAV3 combines an efficient hierarchical tree algorithm for gravity and neighbour finding with SPH optimized for hybrid CPU/GPU architectures. Its hybrid shared/distributed memory model, combined with an asynchronous communication scheme, allows the code to scale efficiently to thousands of CPU cores and GPUs, simulating trillions of particles across thousands of nodes.

Distributed heterogeneous architectures have become a reality in HPC, reaching exascale performance by utilising all available hardware. However, they require decisions about where each task and its data should reside. Persistent GPU data suit interactions and closely coupled CPU–GPU systems also permit cooperative execution using larger host memory. SWIFT's heterogeneous development illustrates this complementary approach [6]. The tree structure is traversed down to groups of 64 particles on CPUs and 256 particles on GPUs, with interactions evaluated via SIMT parallelism on GPUs or SIMD vectorization on CPUs. The grand challenge is to scale such algorithms across distributed nodes while preserving locality and concurrency.

Data management and sustainable software

Memory management is an algorithmic constraint: particle properties, neighbour lists, halo replicas and temporary buffers compete for *finite high-bandwidth* memory. Spatial ordering and suitable field-array layouts can improve locality and coalesced access. Future designs could minimise duplicate represen-

tations across CPUs and GPUs. Memory pools and explicit buffers can reduce allocation overhead and support asynchronous execution. AI-driven hardware development also benefits HPC, but AI favours single (FP32) and half (FP16) precision over double precision (FP64) [10]. SPH could save memory and bandwidth through mixed precision, provided accuracy, stability and repeatability remain proven.

I/O optimisation at exascale extends beyond writing snapshots faster. Parallel output, asynchronous staging and carefully selected fields and cadence can reduce filesystem pressure. SPH-EXA's ADIOS2 and Ascent pipeline demonstrates in-situ analysis and visualisation [7], suggesting opportunities to retain observables rather than every particle state. Data analysis competes with the solver for memory and compute resources, so its cost belongs to the performance measurements.

Code portability must incorporate performance and maintainability across architectures. Examples include MPI, OpenMP, CUDA and HIP [4,5]. Future development may separate numerical formulations from execution and memory backends, evaluating options such as SYCL, Kokkos or OpenMP offload against application needs. The choice of SYCL over Kokkos requires a deliberate architectural decision: Kokkos is a library, making projects dependent on a single implementation, whereas SYCL is an open standard supporting multiple backends as exemplified by SHAMROCK [13]. Abstraction does not remove the issues related to the neighbours list, to memory layout and to task size. Shared verification problems, cross-vendor testing and reproducibility should establish comparable physical results and full-solver performance. Sustainable community software also needs accessible workflows and long-term support for developers.

Energy efficiency should be measured as Watts per million (or 100 million) particles in addition to elapsed time. Studies show that kernel-dependent GPU frequency scaling can reduce energy with limited performance loss [8]. Future power-aware scheduling should exploit the different characteristics of interaction, communication and memory-bound phases. Lower instantaneous power can increase total energy if execution times are prolonged, and comparisons should match physics, accuracy targets, simulated duration and output requirements, and state whether energy covers devices or the whole job.

The literature on SPH in high-performance and heterogeneous computing reveals a field in transition. The foundational insight—that SPH's particle locality maps naturally to parallel architectures—has been thoroughly exploited, yielding mature GPU implementations and sophisticated optimization techniques. SPH local interpolation and moving resolution elements offer opportunities for large free-surface, multiphase and astrophysical simulations and ensembles for uncertainty quantification on emerging HPC systems. Realising them requires joint development of numerics and implementation. GC4 promotes portable, accessible codes and reproducible benchmarks that demonstrate convergence together with complete-workflow scalability, memory use and energy consumption. The contemporary frontier lies not in raw acceleration but in sustainable performance portability.

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Grand Challenge 5 (GC5): Scientific and Engineering Applications

Giuseppe Bilotta, Matthieu de Leffe, Shreyas Joshi

The SPH method has a well-established history of both scientific and engineering applications. Originally developed in the context of astrophysics, SPH has since been applied to a broad range of problems in oceanography and ocean engineering, geophysics and geotechnics, biomechanics and medicine, as well as automotive, aerospace, and other engineering fields. A sample of the extensive literature illustrating the wide scope of SPH applications can be found in the references below.

The aim of Grand Challenge 5 is to promote and strengthen the use of SPH in scientific and engineering applications. This includes developing novel applications in fields where SPH has not yet been widely adopted, and extending existing applications to increasingly complex problems, improving the reliability, relevance, and impact of SPH-based simulations.

GC5 is intentionally broad and application-oriented. It provides a framework for the SPH community to identify, address, and disseminate the scientific and technological challenges arising when SPH is used to study real-world systems. These challenges may concern the complete simulation workflow, from geometry preparation and particle discretization to the extraction, interpretation, and communication of application-relevant results. They may also involve the selection and calibration of appropriate physical models and numerical formulations, as well as the integration of SPH with complementary experimental, analytical, and computational approaches.

A central objective of GC5 is to establish when and why SPH is an appropriate modelling approach. This requires not only demonstrating successful applications, but also critically assessing the accuracy, computational cost, robustness, limitations, and added value of SPH in comparison with alternative methods. Such assessments should be supported, whenever possible, by transparent validation procedures, well-defined benchmarks, uncertainty analysis, and reproducible computational practices.

Scientific and engineering applications both benefit from and motivate advances addressed by the other Grand Challenges. Developments in physical modelling, numerical consistency, stability (GC1), efficiency, adaptivity (GC3, GC4), multiphysics, and multiphase modelling (GC2) are ultimately assessed through relevant application problems. Conversely, application requirements expose limitations, define meaningful benchmarks, and provide motivation for further methodological developments.

For example, industrial applications are driving research on mesoscale and microscale modelling in SPH, including surface tension and contact-line (triple-line) effects, boundary layers and turbulence (GC2). In both industrial and scientific applications, phase change

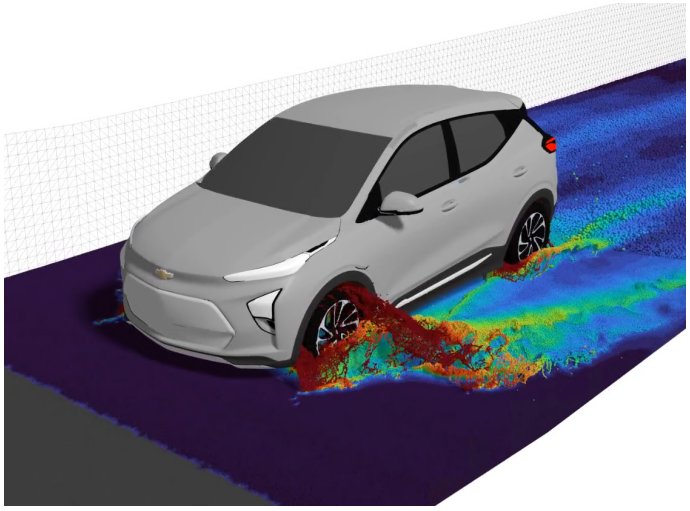


Fig. 1: Example of vehicle wading modeled with SPH. Image courtesy of Siemens Industry Software.

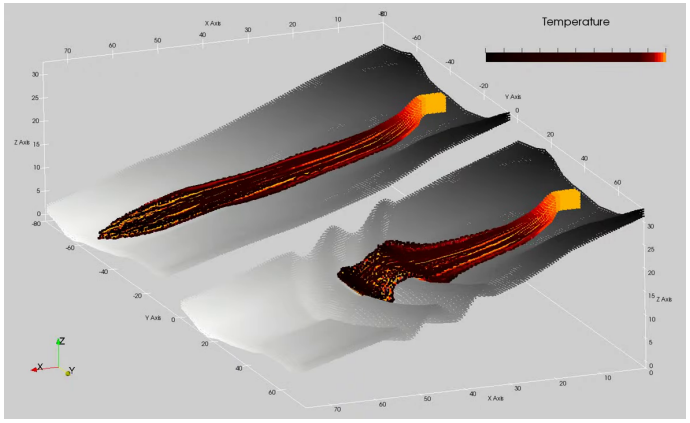


Fig. 2: SPH modelling of a lava flow, showing the effect of ditches and levees in slowing down the flow. Image courtesy of the Osservatorio Etneo, Istituto Nazionale di Geofisica e Vulcanologia.

is a key research area, both liquid/solid and liquid/gas, as are non-Newtonian fluids and other non-linear materials (e.g. viscoelastic, viscoplastic and elastoplastic), especially in geophysics, and in geotechnical and medical applications.

A key aspect of scientific and industrial applications is the integration of experimental and field data. Data assimilation may come into play in industrial design through iterative modelling and incremental design (gearbox lubrication, wading, etc.) and in geophysics (integration of field data in scenario forecasting), with challenges through the whole simulation process, from the pre-processing stage (discretization of complex geometries) to the post-processing (data extraction), and including two-way coupling with other models (such as finite element methods for fluid-structure interaction, discrete element methods for granular flows, or finite volume methods, as often used in the aerospace industry).

Applications often require large-scale simulations involving millions or even billions of particles, making computational efficiency crucial (GC3, GC4). The choice of SPH formulations and models to adopt is therefore often driven by a problem-specific compromise between accuracy and runtime, which may favor less accurate formulations with higher computational performance. Extensive validation and benchmarking are often needed to determine the (Pareto-)optimal balance, and the study of strategies to reduce this preliminary work is also part of the research in GC5.

The ratio of accuracy to computational cost remains a critical criterion in applications both industrial and scientific. Due to its original application in astrophysics, the explicit compressible SPH method, followed by the pseudo-compressible method for free-surface flows, has been extensively studied and developed. Nevertheless, it suffers from a significant limitation on the size of admissible time steps, which has led to the development of the semi-implicit incompressible SPH method, allowing for a significant relaxation of the time-step constraint. The latter method has achieved notable success in industry, demonstrating the method's competitiveness against traditional mesh-based approaches, whereas in scientific applications the weakly compressible formulations remain common, although an implicit treatment of the viscous term is still necessary for flows with very low Reynolds number, as can be found e.g. in geophysics.

The ability to efficiently port these methods to increasingly fast hardware is also a parameter that must be taken into account. For instance, a method that is faster on paper but involves complex numerical operations may prove more difficult to optimize on certain hardware architectures. The Lagrangian nature of the SPH method also leads to less uniform workloads, so that a dedicated framework may be needed to fully leverage the computing power of modern high-performance parallel hardware. This is even more crucial with the adoption of particle refinement strategies, which represent another promising avenue to improve efficiency by allocating computational power more selectively to areas where higher accuracy is required.

These are just a few examples of how Grand Challenge 5 contributes to the virtuous cycle in which scientific advances enable new applications, and application needs guide the evolution of the SPH method. The community can reinforce this cycle by developing application-oriented SPHERIC benchmarks with documented experimental or field data, and sharing tools, input files and datasets to make application results reproducible; publishing assessments of accuracy, robustness and computational costs in application-relevant problems, comparing SPH formulations with one another as well as against other methods, and presenting these results, including limitations and failures, at SPHERIC conferences as well as more application-oriented conferences, can also contribute to this virtuous cycle, welcoming contributions from both academia and industry.

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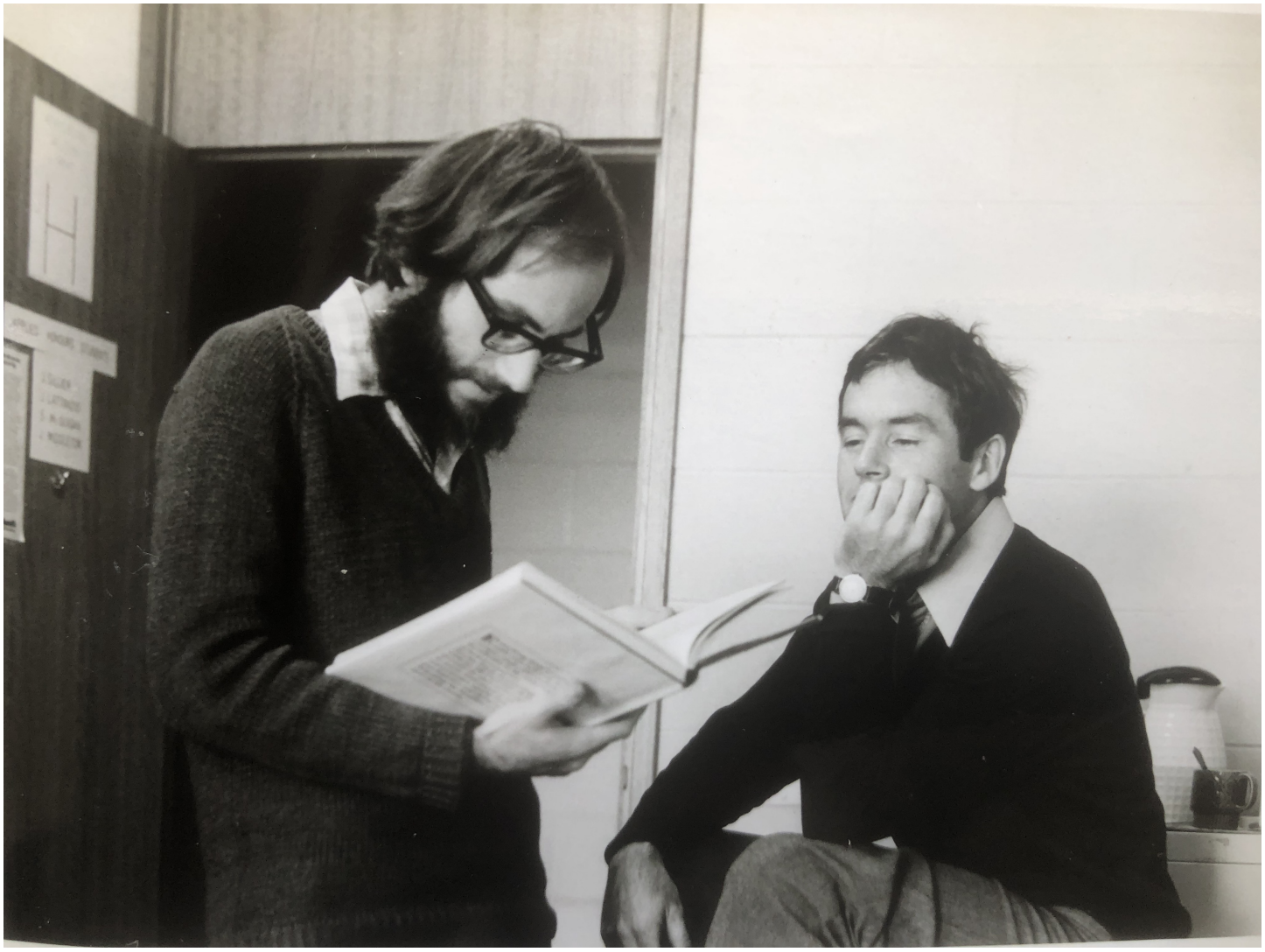
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In photo: Robert Gingold (left) and Joe Monaghan (right) at Monash University, around 1979.
Photo courtesy of Dr. Gingold.

The origins of the Smoothed Particle Hydrodynamics: some reminiscences by Dr. Robert Gingold

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Following our earlier contribution to SPHERIC Newsletter N°40 on the origins of SPH [1], we reproduce here a letter from Dr. Robert Gingold, received on 24 April 2026. In this letter Dr. Gingold describes his personal and academic relationships with Prof. Leon Lucy and Prof. Joseph Monaghan, and offers a fascinating glimpse into the life of the key figures behind SPH in the years surrounding its birth.

Dr. Gingold recalls:

> "I arrived at the Institute of Astronomy (IoA) in Cambridge in early 1976 having completed a PhD in Stellar Evolution at Mount Stromlo Observatory at the Australian National University (ANU). I was planning to continue that sort of work in Peter Eggleton's group at the IoA.
>
> Shortly after I arrived, I attended a seminar by Leon Lucy in which he outlined his ideas about a particle based method. I took some notes, but I did not think of getting involved myself at the time. Leon did not use the term SPH and delivered only one lecture on the subject. He attended a seminar which I gave on my PhD thesis. I recall that he commented on my presentation by saying something along the lines of it involved 'epicycles within epicycles' which I thought was amusing and sadly, probably accurate.

Some time after Leon left, Joe Monaghan arrived from Monash on some sort of sabbatical. He had been one of my undergraduate lecturers at Monash University in Melbourne. Someone at the IoA decided that we should share an office. I used to joke that they wanted to keep us crude colonial Australians quarantined from the rest of the staff.

I told Joe about Leon's lecture. We discussed it and decided to try it ourselves and named it SPH. I don't think at the time either of us were aware of Sanders' work (*Authors' note: see [1] and [4]*). Leon had left well before then. I think he had only been on a short visit.

In late 1977 I visited Leon at Columbia University with my wife. I was a little concerned that Leon might feel we had not given him sufficient acknowledgement in my first SPH paper with Joe, but that concern was immediately dismissed by Leon. He was very welcoming. I recall he was shocked to learn which route we had taken to his office. We had got out at the wrong train station and had to walk through a park. Leon said that the park was notoriously dangerous and we were lucky to survive without being mugged. We discussed SPH for an hour or so. I'm not sure, but I think Leon didn't pursue SPH-type work simply because he had so many other interests.

I then moved to a fellowship at the Department of Physics at the University of Illinois Urbana-Champaign. I continued collaborating with Joe who was back at Monash. Since it was in pre-email days, we exchanged letters frequently. I still have copies of much of that correspondence.

When I returned to Australia I worked with Joe at Monash for a few more years. In 1981 I went back to the ANU as a Senior Research Fellow. I continued SPH work using a vector supercomputer, the CDC Cyber 205 that the CSIRO had installed in Canberra (CSIRO is Australia's national science and industrial research organisation).

This led to a career change for me. I was one of the few people who had managed to use the machine and the CSIRO asked the ANU if I could be seconded to them for a year to help develop the uptake of the technology in their research community.

After I returned to the ANU, the university decided to buy its own supercomputer, the first at a university in Australia and offered me a post of running a small unit of Academic Consultants to research and promote its use. Over time this grew into the Australian national HPC facility with a staff of around 30. It is now a larger organisation housed at the ANU called the National Computational Infrastructure."

Robert Gingold, Emeritus Fellow at Australian National University, Canberra, Australia.

The authors are grateful to Dr. Gingold for contributing this valuable account to their research on the origins of SPH.

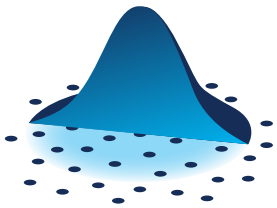
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