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Boundary and Initial Condition Issues for Computational Fluid Dynamics (CFD) and Modeling and Simulation (Mod-Sim)

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Dennis Bushnell

Introduction

For many decades, major Mod-Sim progress has been enabled by improvements in computing machine capability and algorithms; increasingly replacing physical experiments and providing ever improving design and analysis capabilities. Machine speed has improved by many orders of magnitude. Going forward computing will be leaving silicon and shifting to bio, optical, quantum, nano, molecular and atomic computing, with further major improvements expected in the coming decades [ref. 1]. As an example of the Mod-Sim impacts upon physical experiments, NASA Langley has, over the past decades, closed a major proportion of the Center's wind tunnels across the speed range. This is partially due to advances in Mod-Sim, where increasingly we have been able to compute as well as or better than we can measure in wind tunnels. The major wind tunnel requirement still extant is complex turbulent flows. Then there are the huge ongoing efforts in quantum computing. This technology is advancing rapidly and for an increasing number and classes of problems there are projections of truly major performance improvements. Given such capabilities, long held Mod-Sim desires such as direct numerical simulation of turbulence for practical engineering situations in a design mode appears possible.

Given successful development of quantum computing, Mod-Sim would emerge as the winner regarding physical experiments nearly across the board including perhaps even for discovery. Then there is the concurrent development of artificial intelligence, increasingly capable of ideation, to enable Mod-Sim to better optimize designs and predictions. It would thus appear that all is well, with Mod-Sim increasingly capable going forward, resulting in a very bright future. Unfortunately, such is not quite correct for all applications. To execute and apply, Mod-Sim requires initial and boundary conditions (IC/BCs) [refs. 2-5]. The more detailed the computations become, the more detailed the initial and boundary condition requirements become. The Mod-Sim literature appears to concentrate on the solution scheme(s) and at least thus far appears to be paying less than perhaps necessary attention in some cases to the specification of physical/problem-specific initial and boundary conditions, beyond assuring they are mathematically well posed with regard to verification and validation [ref. 6]. What appears to be needed are studies that address the sensitivity of Mod-Sim results for applied engineering and scientific problems to the IC/BC details and their nature, as a function of the physical resolution, for the systems of systems characteristics of real-world problems. As indicated herein, that would result in identifying the need, for various classes of problems, for serious studies and improvements of the IC/BC epistemology and the extent to which the requisite nature and sensitivity of the IC/BCs can be physically specified and realized for problems which are sensitive to such.

Boundary and initial conditions are one source of uncertainty in Mod-Sim [ref. 7], an uncertainty that can be exacerbated in some applications due to the real physical world with all its system of system complexities and variabilities. Other sources of Mod-Sim uncertainty include discretization errors, computational-to-physical micro and macro geometry mismatches, uncertainties in modeling/constitutive relations, truncation errors, and "gridding" [refs. 8, 9]. There are two obvious classes of initial and boundary conditions – postulated, assumed or theoretical and the real world in the systems of systems context. For many problems, the totality of the application conditions can require real world, very detailed, problem specific values which in turn requires study of their epistemic uncertainty, resulting in some cases in a realization of their current virtual unknowability in requisite detail.

There are several classes of problems where major changes result from quite small initial/boundary condition changes. This is studied in the chaos systems literature, where this problem set is one of their defining states (including bifurcations). It is most notorious regarding the issue of sneezing in L.A. affecting the weather on the East Coast at a later date, also known as the infamous "Butterfly Effect" [refs. 10, 11]. A definition and requirement of chaos theory is sensitive dependence upon initial conditions. Then there are systems for which it is either not feasible or currently not possible to measure the requisite nature and details of the initial/boundary conditions. Aside from examples from chaos theory, perhaps the most notorious problem set associated with the importance of low amplitude initial/boundary values is boundary layer transition. Others include multiphase flows, cavitation, atmospheric aerosols, material durability/crack growth, combustion ignition and surface chemistry effects where small numbers of atoms can have major impacts. Sensitivity to initial/boundary conditions has been examined but there have been few studies concerning the issues of knowability from the physical world of such conditions for classes of hyper-sensitive problems. For example, in an observed experimental study of flow separation in shallow circular wall cavities at low speeds, the flow separation patterns experimentally were observed to be asymmetric or skewed to one side. An accidental hit upon the wind tunnel wall flipped the flow pattern to being skewed the other way/side, indicating a bifurcating flow situation.

The Classic Case of The Importance of IC/BCs - Boundary Layer Transition

The transition from laminar to turbulent flow is of great and fundamental importance in fluid dynamic applications. Skin friction drag, heat transfer, and mass transfer can increase by an order of magnitude between laminar and turbulent flow states. The physics of the myriad transition mechanisms have been and are being exhaustively studied, in terms of both linear and non-linear mechanisms. Each have numerous and possibly interacting manifestations depending upon both the details of the physical problem and the IC/BCs. Given a set of initial and boundary conditions and an adequate machine capability transition is predictable. The problem is the multifarious nature of causative initial/boundary disturbance fields [ref. 12] and the minute amplitudes that can affect the dynamics. These disturbance fields arise from both the ambient conditions and from dynamics associated with the particular technical device of interest. In terms of stream disturbance fields, transition prediction requires, depending upon application, specification of ambient particulate fields (e.g., sizes, number densities, geometries, composition), stream temperature spottiness, composition variations, and pressure disturbances. It also includes the spectra and nature of incident dynamic vorticity fields including any organized characteristics thereof, instabilities in thermal (or in the ocean) salinity stratification, internal wave breaking, and embedded shear layers (e.g., the Gulf Stream, the Jet Stream, other currents, benthic and atmospheric boundary layer shear flow turbulence and free surface dynamics effects in the water column).

For aircraft or missiles, particulates can affect transition through many mechanisms, which are dependent upon the particulate details. These mechanisms include direct and dynamic shock distortion, production of particle-produced shocks which strafe the flow and rotation if imbedded within the shear flow, as well as roughness from surface adhesion. Sources of atmospheric particulates include noctilucent clouds (e.g., cosmic dust), residue/emissions from previous rocket launches and aircraft, rain/hail/snow, volcanic activity, solid sulfuric acid from power plant efflux, lofted terrestrial sand/dust, particulates formed from lofted terrestrial natural and anthropogenic bio/other chemicals, and bugs. Vehicles also produce disturbance fields which affect transition. These fields include acoustic fields from propulsion and suction/ejection systems as well as turbulent boundary radiated noise from adjacent surfaces, interacting dynamic shock waves arising from adjacent turbulent flows, formation and discharge of dynamic electrostatic fields formed via tribocharging, and surface and material vibration(s).

Aircraft typically build up a large static electricity charge due to engine and atmospheric particulate impacts, tribocharging, usually discharged at points out on the wing to avoid ball lightning and E-M interference. This can discharge locally, producing high frequency disturbances near the surface. Ground test facilities produce their own unique level and plethora of stream disturbances which affect transition. These include acoustic fields radiated from turbulent tunnel walls, stagnation chamber entropy spottiness that converts to vorticity fluctuations during nozzle expansion, and acoustic parker modes within the test section. In open ocean torpedo transition tests, the entities that live in the water column and suspended particulates directly influenced the transition results.

In addition to the extremely rich, varied nature and number of causative disturbance fields, there is the issue that transition occurs due to exponential amplification of extremely small disturbances, often by factors of thousand(s) fold. Since transition results in flows with disturbance amplitudes in the range of 5% plus, knowledge of initial disturbance fields is required for amplitudes beginning in the range of .005% or less. This requires extreme care and excellent measuring equipment for the entire spectrum of varied disturbance field sources, physics and dynamics, including air traffic wakes. For aircraft applications this is required as a function of latitude, longitude, altitude, and time along the flight path. Such a requisite dynamic/initial condition requirement for accurate Mod-Sim transition prediction as an initial/boundary layer problem in meaningful ways does not exist, and it may never exist. Vehicle-induced disturbance fields are various and vehicle and vehicle operation specific. Their effects are modified by the huge parameter space(s) that affect transition including details of flow history and local flow conditions. In laminar flow control flight tests, a greater than 50-mile visibility was required to avoid the effects of atmospheric particulates upon system performance [X-21 Project, ref. 13]. Bug impacts upon the leading-edge region during takeoff had to be designed around (or aircraft flown when outside temperatures were cool to minimize bugs, e.g., early in the morning). Overall, differences in these ambient and variable vehicle-induced disturbance fields can result in large changes in boundary layer transition location. The transition location can be critical for design of wing leading edges/high lift/ laminar flow control, unmanned aerial vehicles (UAVs), GA aircraft, empennage, gas turbine engine blades, propellers, nacelles, and missiles across the speed range.

IC/BCs for Multiphase Flows

Multi-phase flows [ref. 14] are notorious in terms of predictability problems/issues [ref. 15 - 17], especially cavitation and boiling. Alterations in the adsorbed gas content in the liquid column, details of particulate loadings, changes in surface morphologies, and surface chemistry (often altered by small numbers of atoms), etc. affect, in often major ways, the occurrence and predictability of multi-phase flows. The situation can be serious. Chemical processing plants can involve multi-phase flows and scaling can be difficult from pilot to full scale plants due to issues with predictability of multi-phase flows. This leads to conservative designs and possibly design failures for full scale expensive plants. From aircraft icing research, the requisite initial boundary condition requirements include details regarding distribution and characteristics, sizes of particles and droplets in free stream and clouds, cloud and free stream temperature distributions, and cloud and free stream moisture content [ref. 18]. Machine limitations currently require constitutive modeling of particle agglomerations, which are sensitive to details of individual particle material(s), geometry(s), electrostatics, etc. Ignition delay [ref. 19] is a critical issue in combusting system design and operation. Presence of trace chemical contaminants, free radicals, and condensed and/or charged and excited species can alter ignition delay/behavior by 10X or more. What is needed are detailed measurements at levels capable of having a first order effect. Mod-Sim for arcing and breakdown in gases [ref. 20] requires details of electrode surface morphology, corrosion and adsorbed contaminants, details regarding particulates embedded in the gas, and details of gas contaminants and composition including moisture.

The MOD-SIM Asymmetric Nose Vortex Problem

Missiles at angle of attack often exhibit asymmetric nose region vortices which produce large unintended side forces [ref. 21]. The mystery of their occurrence has not been fully solved but observed sensitivities include triggering by often imperceptible geometry differences including tool marks, slight skewness in free stream, and dust deposits both initial and acquired during testing/flight that are deposited from the free stream. This occurs in both laminar and turbulent flow, but asymmetric transition is a further cause. Then there is the often-exquisite sensitivity to extreme details of the bounding surface geometry. Discontinuities in second derivatives of the surface geodesics can generate longitudinal vortices.

MOD-SIM for Climate and Aerosols

Aerosol effects on climate are the same order as, but opposite in sign to, CO_2. Key data required to effectively conduct atmospheric aerosol Mod-Sim [ref. 22] includes distributions/levels of:

- Cloud condensation nuclei
- Droplet size spectrum
- Electric charge distributions
- Chemistry, including trace species for surface chemistry evaluations
- Turbulence spectra
- Temperature
- Pressure
- Density
- Phase
- Aerosol/particle constituents including black carbon
- Biologics
- Thermal radiation spectrum
- Mean distance between drops
- Ice particle geometries

The requisite climate change estimates going forward decades requires computation or measurement of these aerosol inputs, which in turn requires exquisite knowledge of their sources and boundary conditions. This involves a vast number of interacting processes, including terrestrial.

Effects of Surface Morphology on Atmospheric Boundary Layers

The details of surface morphology and other surface conditions can affect the atmospheric boundary layer. Experiments involving addition of oil to alter sea surface wave details with subsequent downwind boundary layer measurements indicates that suppression/alteration of small-scale wave dynamics significantly alters the atmospheric turbulent boundary layer at sizable altitudes. This indicates sensitivity to details of the entire surface dynamic wave motion spectrum. Soil moisture details are essential for atmospheric boundary layer computations over complex terrain. This necessitates detailed knowledge of subsurface morphology, conditions, and dynamics [ref. 23]. Atmospheric boundary layer development over urban terrain requires details regarding the roughness elements (e.g., buildings, etc.) and their mass and thermal/chemical exchange boundary conditions [ref. 24].

Boundary Conditions Required in Fire Modeling

Fire is a three phase fluid dynamics problem with complex chemistry and geometry. Knowledge of the physical distribution and composition of the materials is required along with their variegated physical state, as locally affected by drying, sun exposure/aging, etc. Details of the wind turbulence condition and air moisture content are also required, along with aerosol details, terrain, and surface morphology [ref. 25, 26].

Boundary Conditions Required for Riverine System(s) Mod-Sim

Detailed computation of riverine systems requires knowledge regarding water sources/sinks (e.g., streams, rainfall, outflows, solar forcing). It also requires mapping of bounding soil characteristics (e.g., roughness, porosity, saltation and sediment adhesion, saturation). In addition, bounding surface topology, including curvatures which instigate Gortler Instabilities and in the limit, presence, types, behaviors of burrowing, and damming wildlife [refs. 27 – 29].

MOD-SIM for Fracture, Fatigue, and Durability

Material fabrication typically induces distributed residual stresses, heterogeneous grain typography, dislocations, oxide films, pores, and poly-crystals, among other ultra-small scale inhomogeneities that affect, to first order, crack initiation and growth [refs. 30, 31]. Currently missing is adequate data with regard to 3-D grain structure, inclusions, dislocation substructures within grains and residual stress distributions required, batch by batch, for prediction of fracture, fatigue, and durability. Corrosion damage and its predictability in aluminum alloys is the direct result of local galvanic coupling between constituent particles and the metal matrix. To predict damage evolution accurately in three dimensions, the spatial distribution (and nature) of the constituent particles (i.e., contaminants – crushed particles throughout the matrix) in a given material must be quantified. Related to this materials damage Mod-Sim boundary/initial conditions unknowability shortfall is the prediction of earthquakes and explosions in mines, which require a knowledge of detailed geological details (aka materials, structural morphology, and gases) currently unavailable.

The Case of Surface Chemistry Effects

Surface chemistry [refs. 32, 33] is increasingly important in nano, surfactants, adsorption, adhesion, catalysis, lubrication, corrosion, and other technologies going forward. This field has been termed "the closest thing to magic" that exists. Small concentrations of constituents can have major effects. It requires the measurement/knowledge/specification of the presence/amounts of operable trace constituents. One of the great challenges of surface chemistry is the intrinsic difficulty of experimentally measuring surface structure. This stems from the extremely small number of atoms at the very surface that controls surface reactivity.

Micro-Gravity Mod-Sim Boundary Condition Issues

Surface-tension-driven flows in micro-gravity conditions are zeroth order dependent upon the condition of the surface. Oxide formation, or other surface reactions and contamination due to dust and contaminants in the environment or apparatus, can inhibit or even eliminate surface-tension-gradient-driven flows [refs. 34, 35].

Mod-Sim for Removal of Contaminants from Soils by Electrokinetics

What is required to remove contaminants from soils using electrokinetics are pH and surface chemistry of the soil, knowledge of details concerning and electrochemistry of all contaminants, hydrological properties of the soil, and electrode details. [ref. 36].

Some Hypersonic Boundary Condition Issues

Surface catalysis for finite rate chemistry is affected by wall porosity/adsorption, roughness, material heterogeneity, and handling/exposure. For low density/high altitude flows, slip boundary condition distributions are affected by environmental exposure(s).

Boundary Condition Issues with Regard to Air Quality Computations

Air pollution (including ozone computations) require extensive initial conditions and detailed dynamic boundary conditions. The latter is driven by the often-dynamic nature of neighboring winds and industrial activities. Evidently, it is currently not feasible to measure the requisite IC/BCs given the necessary resolution and the dynamic and complex nature of constituents and conditions in the atmosphere [refs. 37, 38]. One possibility is to develop and utilize smart dust sensing, which in millimeter sized dust motes includes energy harvesting, sensors, navigation, and optical communications. The issue is they would also constitute pollution so a multiplicity of fixed optical sensors scanning the computational and boundary zone at high repetition rates is a more probable solution space.

A Summary of the Outlook, Need for, and Improved Knowledge of Initial/Boundary Conditions

For Sensing - Development/deployment of nano and quantum sensors, deployment/networking of a global sensor grid, including utilization of energy harvesting with machine intelligence for sense making.

“Sensors are poised on the brink of a revolution similar to that experienced in micro-computers in the 1980s.”

-Jon Wilson, 2004
Editor-in-Chief, Sensor Technology Handbook

For many important classes of Mod-Sim problems, even quantum computing will not enable accurate predictions/computation vis-à-vis the real world due to boundary/initial condition shortfalls in terms of both range of parameters and requisite amplitudes/coverage.

Overall, the Mod-Sim community must become much better educated with regard to the physics, experimental aspects, and sensitivities of the problems addressed including the importance and knowability of initial and boundary conditions.

The current situation in most of Mod-Sim involves/requires the utilization of phenomenological/heuristic modeling of very complex physical processes, often using lumped parameter constitutive relations. As the machines allow the direct computation of these generally smaller scale and complex dynamical system physical processes which are now modeled, **<u>this physical/boundary/initial specification shortfall will become both far more prevalent and far more critical.</u>** As an example, over the past three decades the greatly improved machine capabilities have enabled boundary layer transition prediction to move from wholly problem specific and unsatisfactory empirical transition Reynolds numbers, to the capability to compute the receptivity, linear, and nonlinear transition processes. Such requires specification of initial/boundary conditions for application, which we do not have.

Some possible issues to consider depending upon application include:

- Material aging effects
- Surface chemistry
- Contaminants of all flavors/characteristics including particulates
- Bifurcating flows and their sensitivities
- Surface morphology, including geodesics/2nd derivatives and roughness of all flavors
- Exponential amplifications triggered by initial/BCs, path dependent phenomena
- Physics/sensitivities to dynamic Initial and boundary conditions

For design, we often need far more definitive results than mere probabilistic forecasts of solution space variability based upon maximum parametric excursions. These often exhibit variabilities that preclude successful design spaces.

We need physical data-The computational specialist has really no choice in many cases/problems and needs to **interact with the REAL WORLD**. Real world knowledge shortfalls will limit the usability/value of an increasing number of ever more detailed applications of Mod-Sim going forward.

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For many important classes of Mod-Sim problems, even quantum computing will not enable accurate predictions/computation vis-à-vis the real world due to boundary/initial condition shortfalls in terms of both range of parameters and requisite amplitudes/coverage. The Mod-Sim community needs to consider going forward the knowability of initial and boundary conditions.

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