Epistemic Issues Concerning Boundary & Initial Conditions in MODSIM

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Some Problem Class Specific Experimental Epistemic Issues Which Bode Ill for the Futures of CFD…….

“The ability to Quantify uncertainty in large scale computations is THE missing piece of the puzzle” [Tim Barth, NASA-ARC]

MODSIM Sitrep - 1

- MODSIM is, in real time, replacing Physical Experiments and increasingly providing ever improving design and analysis capabilities
- This progress has been enabled mainly by the exponential improvements in Machine Capability , aided by algorithm advancements
- Machine speed is now some E8 greater than in the late 50’s, on Silicon. Going forward we will leave silicon and go to Bio, optical, quantum, nano, molecular & Atomic computing, With an additional E8 to E12 improvements expected in the coming decades

NASA Langley has, over the past two decades, closed a major proportion of the center "Wind Tunnels" across the speed range, partially due to advances in Mod-Sim

MODSIM Sitrep - 2

- Quantum computing is “Different”, the technology is advancing rapidly and for an increasing number / classes of problems there are projections of up to some E44 better performance. Given such speeds long held ModSim “Maidens Prayers” such as Turbulence DNS for practical situations in a DESIGN mode appears probable.
- Given Quantum Computing MODSIM appears to emerge as the “Winner” wrt Physical experiments across the board including perhaps even for “Discovery”

MODSIM Sitrep - 3

- The machines are currently running at essentially human brain speed [~ 20 Pflops], with, as indicated, much greater in the offing.
- There are 3 major approaches to attaining Human level Machine Intelligence, Soft Computing, Biomimmetics and Emergence. Of these Biomimmetics [nano-sectioning the Brain and replicating in Silicon] appears to be the closest in, with the IBM Blue Brain Project and now others projecting some 10 years out.
- Given even the runup to human level machine intelligence the machines are/ will become capable of the ideation function as well as the analysis/ design functions.

[Example] - Automated Invention

- Steve Thalers’ Creativity Machine AKA Imagination Engine
- A trained neural net is deprived of all rational input
- “Dreams”, apparently as people dream, producing multitudinous new combinations/”ideas”
- A “critic” neural net evaluates these ideas for various problems/metrics
- Quite successful, good “Track Record”, many other such………NOW

MODSIM Sitrep - 4

- It would thus appear that All is WELL, MODSIM Uber Allis, very BRIGHT Future, just need to work the problem[s]…….

UNFORTUNATELY, such is not quite Correct. To execute/ exercise MODSIM require **<u>Initial and Boundary Conditions</u>**. The MODSIM literature appears to concentrate on the solution scheme[s] and pays little serious attention to initial and boundary conditions, The computational folks largely appear to assume these will , somehow, appear/ BE THERE, via immaculate conception or otherwise, they appear to largely care not, most simply assume is a “detail” and most are simply not familiar with the physical world to the extent required to “Make good Numbers”.

Computability and Uncertainty in MODSIM

- Boundary and Initial Conditions are one source of "uncertainty" in ModSim
- Other sources of Uncertainty include such as Discretization Errors, Aeroelastic Distortions, Computational-to-physical micro and macro geometry mismatches, uncertainties in modeling/ constitutive relations, truncation errors, "Gridding"
- Usually addressed if addressed via various Probabilistic and more recently non-probabilistic / "Fuzzy" approaches, often neither considered nor addressed

Many of the major works on Uncertainty in CFD are due to ICASE/ICASE [under Hussaini] and folks related thereto. Y. Hussaini is an author on several of these.

E.G. - From ICASE Report 2001-35 [For a Burgers Equation model] "Ignoring this boundary condition uncertainty dramatically underestimates the variance of the velocity in the interior of the domain"

“Given a Perfect Model, predictability is limited only by the growth of the uncertainty in the initial condition”

SMITH ET AL, 1999

Boundary and Initial Conditions - 1

- There are two obvious flavors of Initial and boundary conditions – Postulated/assumed/theoretical and the REAL WORLD
- The former addresses/ concerns issues such as truncated regions, outflow conditions, absorbing walls, etc.
- This Presentation briefly examines the issues associated with REAL WORLD specification of Initial and Boundary Conditions, termed Epistemic Uncertainty

Boundary and Initial Conditions - 2

- There are several classes of Problems wherein the important/ critical phenomena/physics are rapid-to-exponential, and/or where major changes result from quite small initial/boundary condition changes. This is perhaps best studied in the Chaos/Dynamical Systems Literature, where this problem set is one of their defining states, including bifurcations, and is most notorious wrt the issue of sneezing in L.A affecting the weather on the East Coast at a later date, the infamous "Butterfly Effect"……..

One definition/ aspect/requirement of Chaos Theory is defined as “Sensitive Dependence upon Initial Conditions”

Three Classes of “Unpredictable” Problems

- Systems that are hypersensitive to initial conditions [considered in Chaos Theory]
- Systems for which we lack constitutive equations/ the “physics” etc.
- Systems for which it is either not feasible or currently not possible to measure the requisite nature and details of the initial/ boundary conditions, termed by Jan Hesthaven The “Unmeasurable Parameters” problem

Boundary and Initial Conditions - 3

- [Aside 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 such as multiphase flows, cavitation , atmospheric aerosols, material durability/ crack growth, combustion ignition etc., also surface chemistry effects where small numbers of atoms can have major impacts
- Sensitivity to initial/ boundary conditions has been examined but not so much the issues of “knowability”, from the physical world, of such conditions for these classes of hyper-sensitive problems.

An Example of Boundary and Initial Condition Issues in Bifurcating systems

- In experimental studies of flow separation in shallow circular wall cavities the separation patterns have been observed to be asymmetric, skewed to one side. An accidental hit upon the wind tunnel wall flipped the flow pattern to being skewed the other way/side………

In the following Presentation continually ask yourself “How Much of this requisite Initial/ Boundary Condition Information will we know and WHEN [years hence] will we know it. If we will not know it, what would be the effect upon the efficacy of Mod-Sim, what are the “work-arounds” to a cogent Mod-Sim Solution space

Boundary Layer Transition Sensitivity - 1

- The transition from laminar-to-turbulent flow is of great and fundamental importance in fluid dynamic applications. Typically skin friction drag, heat transfer and mass transfer 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 of which have numerous and possibly interacting manifestations depending upon both the details of the physical problem and THE INITIAL/BOUNDARY CONDITIONS.

Boundary Layer Transition Sensitivity - 2

- Given a set of initial and boundary conditions transition, given adequate machine capability, transition is “predictable”. The problem is the multifarious nature of causative initial/boundary disturbance fields and the minute amplitudes which can affect the dynamics. These disturbance fields arise from both the ambient flight conditions and from dynamics associated with the particular technical device of interest.

Boundary Layer Transition Sensitivity - 3

- In terms of stream disturbance fields, transition prediction requires specification of ambient particulate fields [sizes, number densities, geometries, composition], stream temperature spottiness, composition variations, pressure disturbances and the spectra and nature of incident dynamic vorticity fields including any organized characteristics thereof.

Sources of Stream Dynamic Vorticity, Atmosphere and Ocean

- Instabilities in thermal or [in the ocean] salinity stratification, Internal wave breaking
- Imbedded shear layers [e.g. the Gulf Stream, The Jet Stream, other "currents"]
- Benthic and atmospheric boundary layer shear flow turbulence
- Free surface dynamics effects in the water column

Ambient Particulate Example – B.L. Transition

- For Aircraft or missiles, particulates can affect transition through many mechanisms, which/what dependant 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, Also “roughness” from surface adhesion
- Several Missiles, nominally identical, exhibited variable transition behavior apparently caused by differences in atmospheric particulate loading.

Sources of Stream Particulates

- Noctilucent clouds [cosmic dust]
- Residue 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
- "Bugs"

Boundary Layer Transition Sensitivity - 4

- Vehicles also produce disturbance fields which affect transition, these 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 via “tribo-charging”, surface/ material vibration[s],

Electrostatics Example - B.L Transition

- There were several Missile tests with various types of surfaces. One surface was conducting, was very smooth and had delayed transition. Another had a largely non-conducting surface, same smoothness, this one had early transition, presumably due to electrostatic buildup and discharge – at Khz to Mhz. Aircraft typically build up a charge of 600,000 volts or so due to engine and atmospheric particulate impacts, usually discharged at “points” out on the wing to avoid ball lightening/ E-M interference.

Test Facility Disturbance Fields

- 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 region entropy spottiness that converts to vorticity fluctuations during nozzle expansion, acoustic parker modes within the test section, Etc. In open Ocean torpedo transition tests the “critters” that live in the water column and suspended particulates directly influenced the results.

Boundary Layer Transition Sensitivity - 5

- In addition to the extremely rich/varied nature/ number of causative disturbance fields there is the issue of transition occurring 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 is required for disturbance fields with amplitudes in the range of .005% or less., requiring extreme care and excellent measuring equipment, for the entire spectrum of varied disturbance field sources, physics and dynamics.

Sitrep – Boundary Layer Transition MODSIM

- The requisite dynamic/ initial condition panoply to utilize/rely on transition MODSIM in meaningful ways does not exist, and it may never exist. The atmospheric conditions are a function of latitude, longitude, altitude and time including the season[s], along with "traffic" [wakes]. Vehicle-induced disturbance fields are various and vehicle and vehicle operation specific, and their effects modified by the HUGE parameter space[s] that affect transition [DETAILS of Flow History and local flow conditions] as captured by MODSIM.

In LFC Flight tests, a greater than 50 mile visibility was required to avoid the effects of atmospheric particulates upon system performance [X-21 Project]. Bug impacts upon the leading edge region during takeoff had to be designed around [or fly when is cool to minimize bugs]

Overall – Differences in Ambient Disturbance Fields Result in Order[s] of Magnitude changes in Boundary Layer Transition Location, critical for [Examples]:

- Wing Leading Edges/ High Lift/ LFC
- UAV's, GA Aircraft
- Empannage
- GTE "Blades", Propellers
- Nacelles
- Missiles across the speed range

MODSIM for Multi-Phase Flows

- Multi-phase flows are notorious in terms of Predictability problems/issues, especially cavitation and boiling. Minute alterations in the adsorbed gas content in the liquid column, extreme details of particulate loadings, exquisite changes in surface morphologies and "surface chemistry" [often altered by small numbers of atoms] as well as electrostatic fields all affect in often major ways the occurrence and predictability of multi-phase flows. The situation is actually quite dire, most chemical processing plants involve multi-phase flows and it has proven extremely difficult to scale from pilot to full scale plants due to issues with predictability of multi-phase flows, leading to conservative designs and sometimes design failures for full scale, EXPENSIVE plants.

Aircraft Icing Initial/ Boundary Condition Requirements

- Distribution and characteristics/ sizes of particles and droplets in free stream/ clouds
- Cloud/ Free Stream Temperature Distributions
- Cloud/ Free Stream Moisture content

Fluid-Particle Flows

- Details of Surface Chemistry important-to-critical, e.g. “chaining” of particles to produce friction reduction
- Machine limitations currently require constitutive modeling of particle agglomerations, which are sensitive to DETAILS of individual particle material[s], geometry[s], electrostatics etc…..

MODSIM for Combustion Ignition

- Ignition delay/ ignition is a critical issue in combusting system design/operation. In-stream/ presence of trace chemical contaminants, free radicals and condensed and/ or charged and excited species can alter ignition delay/ behavior by 10X or more. Need detailed measurements of all such at levels capable of having a first order effect.

Mod-Sim for Arcing/ Breakdown in Gases Requires:

- Details of Electrode Surface morphology, corrosion and adsorbed contaminants
- Details of particulates embedded in the gas
- Details of gas contaminants and composition including “Moisture”

The MODSIM Asymmetric Nose Vortex Problem

- Missiles at angle of attack often exhibit asymmetric nose region vortices which produce huge unintended side forces
- 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, deposited from the free stream. 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.

MODSIM for Climate/Aerosols

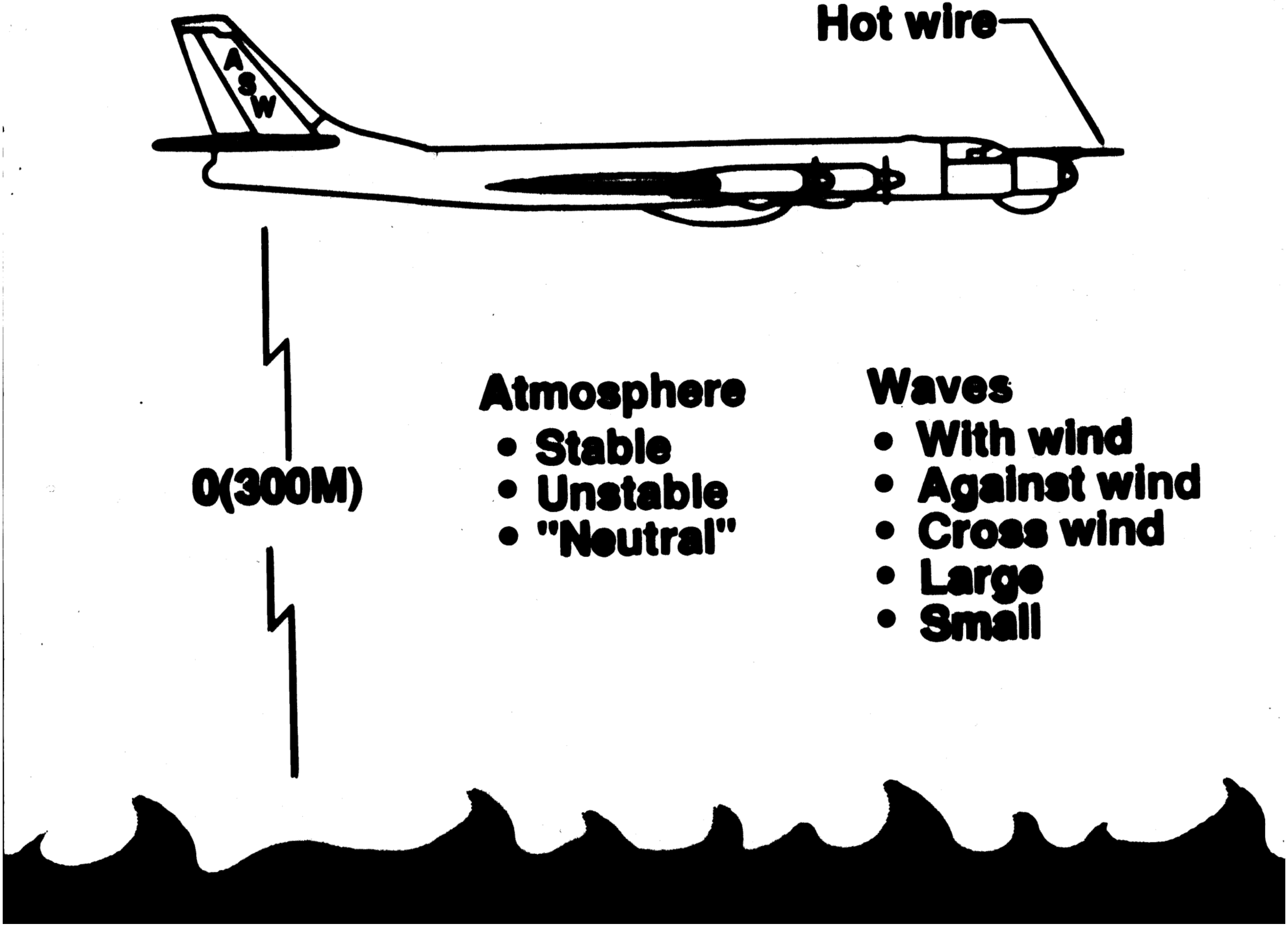
- Aerosol effects on Climate are the same order as but opposite in sign to CO_2
- Key data required to effectively conduct Atmospheric Aerosol ModSim includes distributions/levels of:

- Gas Phase Volatile Organic Compounds
- Anisotropic Micro-scale turbulence
- Trace gas Constituents incl. HNO_3
- Static electric fields
- "Surface active" constituents

The requisite Climate Change estimates going forward decades requires computation of these Aerosol “inputs”, which in turn requires exquisite knowledge of their sources and boundary conditions, involving a vast number of interacting terrestrial processes

Mod-Sim for Atmospheric Boundary Layers Over Water

- Controlled experiments involving addition of oil to alter 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, Indicating sensitivity to details of the entire surface dynamic wave motion spectrum


Hot wire
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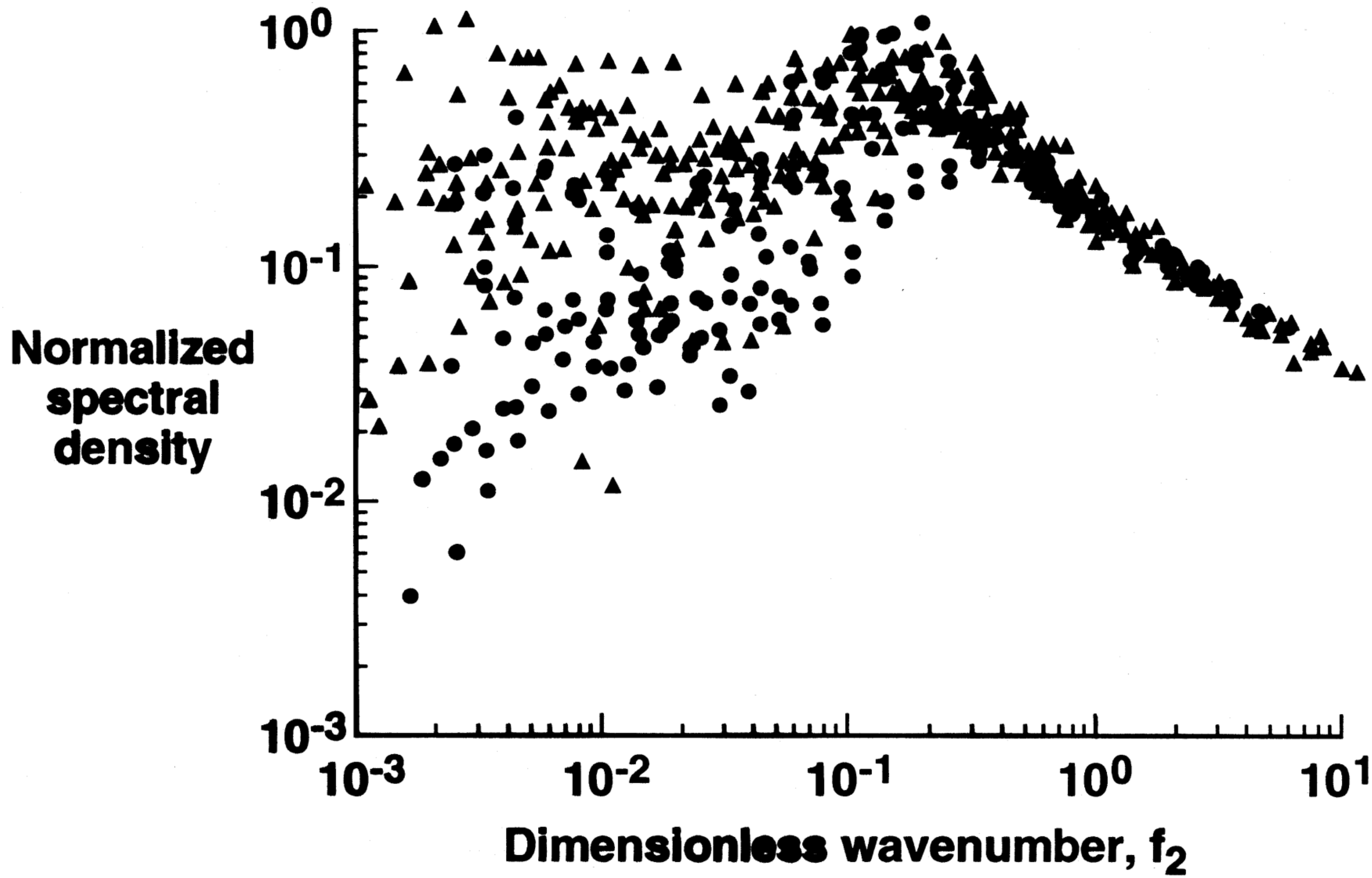

10^0
10^{-1}
10^{-2}
10^{-3}
Normalized spectral density
10^{-3}
10^{-2}
10^{-1}
10^0
10^1
Dimensionless wavenumber, f_2

B.C.s in Fire Modeling

- Varigated ‘Physical State” of the materials required, as affected by drying, sun exposure/ aging etc
- Detailed Physical Distribution and “nature”/ composition of the Materials required
- Details of the wind turbulence conditions and air moisture content required
- Particulate/Aerosol details required

Required for Riverine System[s] Mod-Sim

- Detailed knowledge regarding all water sources/ sinks [streams, rainfall, outflows, solar forcing]
- Complete mapping of bounding soil characteristics [roughness, porosity, saltation/ sediment adhesion, saturation]
- Bounding surface topology, including curvatures which instigate Gortler Instabilities
- Presence, types, behaviors of burrowing and "daming" wildlife

- "There is a Fundamental limitation upon model predictive ability due to problems in specifying topographic complexity"

MODSIM 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.
- Currently “missing” is adequate data wrt 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 [Contaminants – crushed particles throughout the matrix] in a given material must be quantified.”

Related to this Materials damage MODSIM boundary/ initial conditions unknowability shortfall is the prediction of Earthquakes and explosions in mines, which require a knowledge of geological [AKA Materials and Gases] details currently unavailable.

"Surface Chemistry" is increasingly important in Nano, surfactants, adsorption, adhesion, catalysis 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. Requires the measurement/ knowledge/specification of the presence/ amounts of such 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 dependant upon the “Condition of the Surface”. “ Oxide formation or other surface reactions and contamination [due to dust and contaminants in the environment or apparatus] may seriously inhibit or even eliminate surface-tension-gradient-driven flows” [Ostrach, 1982]

Required for Mod-Sim of Removal of Contaminants From Soils by Electrokinetics

- pH and surface chemistry of the soil
- Knowledge of details concerning and Electrochemistry of all contaminants
- Hydrological properties of the soil
- Electrode Details writ large

Entry, Descent and Landing into Mars

- Vehicle dynamics/ associated Aero Computations wholly dependant upon knowledge of the Free stream conditions, including DENSITY
- The knowledge of the variability/ variations of Martian Atmospheric Density is extremely sparse at best, affected by seasonal , diurnal, solar changes and dust storms, Definitive bounding limits not available throughout the altitude range. Variations of 100% have been observed.

“Trace Constituent[s] play a critical role in Planetary Atmospheres….A minor component of the primordial atmosphere, ammonia, together with its trace products was responsible for the atmosphere of nitrogen we have on Titan and Earth today and for the nitrogen component of Venus and Mars Atmospheres”

Some Hypersonic B.C. Issues

- Surface Catalysis for Finite Rate Chemistry [as affected by wall porosity/ adsorption, roughness, and material heterogeneity and handling/exposure]
- For Low Density/ High Altitude flows, “Slip Boundary Condition[s]” distributions, as effected by environmental exposure[s]

The Outlook – Improved Knowledge of Initial/ Boundary Conditions

- Development/ Deployment of Nano Sensors
- Deployment/ Networking of a Global Sensor Grid
- Machine Intelligence for “Sense Making”
- The changing “Art of the Possible”

"Sensors are poised on the Brink of a Revolution Similar to that experienced in Micro-Computers in the 1980's"

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

Sample Characteristics of Emerging Global Sensor Grid

- **Military,Commercial/Industrial,Public Safety,Scientific, Populace Contributions/Observations**
- **Ever-Improving Sensitivity,Resolution, Ubiquity, Connectivity,Fusion/"Sense-Making",Physical Phenomena "Coverage",Persistent & Pervasive…**
- **Land,Sea,Air,Space,"Internal"/External**

- We are "Instrumenting the Planet"

Sample Data Sources - Emerging Global Sensor Grid

[Everything becoming a sensor]

- Safety/Security/Environ. Sensor Nets
- Smart buildings & roads,other smart Infrastructures
- “Overheads”/Sats
- Cell-phone sensors
- Mini-Cams
- Smart Appliances, clothes,other smart “Products” [e.g. Shoes]
- Military sensor nets
- RFID/Nano Tags
- Near Space [75K-350K ft sensors]
- Sensors on transportation devices
- Bio sensors including in situ/in vivo/”toilets”
- Scientific sensor nets
- Populace observations & contributions communicated via internet

Global Sensor Grid Outlook

- We are currently networking some 5-10 million sensors
- The projections indicate in some 10 years we will deploy/ network some 2 Trillion sensors

This WILL NOT begin to TOUCH most of the MODSIM Initial/ Boundary condition issues discussed herein. However, the effort will provide requisite technologies/ enable greater “progress”

Concluding Remarks

- For many important classes of MODSIM Problems even E44 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 MODSIM Community should-to-must become much better “educated” wrt the “physics” and experimental aspects and sensitivities of the problems addressed including the importance and “knowability” of initial and boundary conditions.

The current sitrep 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", **this physical / boundary/ initial specification shortfall will become both far more prevalent and far more critical.**

As an Example:
Over the past 2 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 and linear and non linear transition processes. Such REQUIRES SPECIFICATION of Initial/ Boundary Conditions WHICH WE DO NOT HAVE.
"We have met the Enemy and they is us"

Issues to Consider/ Worry About

- Material “Aging” Effects
- Surface Chemistry/ Energy
- Contaminants of all flavors/ characteristics including particulates
- Bifurcating flows and their sensitivities
- Surface Morphology, including geodesics/ 2^{nd} derivatives & “roughness” of all flavors
- Exponential Amplifications triggered by initial/ BC’s, Path dependant phenomena
- Physics/ Sensitivities to [dynamic] Initial & Boundary Conditions

For Design, 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.

Need Physical DATA, The Computational specialist has really no choice in many cases/ problems, need to **interact with the REAL WORLD**. REAL WORLD knowledge shortfalls will limit the useability/ value of Mod-Sim going forward…