Proposed Checklists for use as one develops the model and the data analysis

These are the in-house checklists used for the UW Model Repository at www.physiome.org
The pages are: 1.Summary 2.Project file, 3. CODE, 4.Verif, 5. Valid, 6. Uncertainty, 7. Publication
The check list is to be used by the author and two reviewers, before approval for website.

	STANDARDS.1.SUMMARY: Summary of Expectations	Auth	Check 1	Ch 2
Group 1: Identification and Description		x		
	1. Model Name and No: short and long descriptions complete		xy	
	2. Code completed, checked .mod file, Model runs correctly			xyz
	3. Diagrams correct			
	4. Reference to Publication describing the model			
	5. Context and Purpose of model defined			
Group 2. Project File: Basic Content: FIGURES and NOTES				
	1. The chosen model solutions tell some story			
	2. The story is around data, figures and parameter sets (All matched)			
	3. The figures and their titles fit story			
	4. Every figure has axes labeled with symbol, name and units			
	5. Figures use Very short tab labels fitting the topic.			
	6. Graphs use same colors and line types for same variable in every figure.			
	7. Sensitivity functions. How to plot. Why useful. Notes. Use same colors.			
	8. Ontology consistent in notation of .mod, Figures and Notes and Par sets			
	9. Notation consistent with diagrams in .mod text and on the Website			
	10. Parameters sets: Description and rationale for each explained in Notes			
	11. Loops: Purposes and settings; parameter set, plus explanation in Notes			
	12. Optimization re data or other model: description, par set, Notes			
Group 3. Verification methods: See STANDARDS-VERIF for detail				
	1. Under Notes: Check off list for the model file verification (X re 10in Gp 3)			
	2. List variables computed in the MML code that are serving as checks			
	3. Commentary on checks or missing checks			
	4. Numerical Methods chosen and why. In notes.			
	5. Solution times chosen; delta t chosen; comments			
Group 4. Validation methods: See STANDARDS-VALID for detail				
	1. Justify initial and boundary conditions in accord with physiology			
	2. List Data provided and fitted by model, and sources.			
	3. Show fits of data in Figures, and optimization results			
	4. Notes defining contents of each situation, figure or par set			
	5. Parameters estimated and evaluated against literature or other			
Group 5. Uncertainty Quantification: See STANDARDS-UQ for detail				
	1. Parameters and Variables chosen			
	2. Define Measures of uncertainty			
	3. Plots or contour maps of projected results			
Group 5: Scientific Publication: See STANDARDS-PUB for detail				
	1. Summary of the science			
	2. References to subsequent publications or alternative models			
	3. Website for public dissemination, commentary and responses			

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	STANDARDS 2: The PROJECT FILE: code, data, etc.	Auth	2nd	Note
Group 1: Identification and Description		x		
	1. Model Name and No: short and long descriptions complete		xy	
	2. Code completed, checked .mod file, Model runs correctly			xyz
	3. Diagrams correct			
	4. Reference to Publication describing the model			
	5. Context and Purpose of model defined			
	6. Provenance: Refs to prior works			
Group 2.Project File: Basic Content FIGURES and NOTES				
	1. The chosen model solutions tell some story			
	2. The story is around data, figures and parameter sets (All matched)			
	3. The figures and their titles fit story			
	4. Every figure has axes labeled with symbol, name and units			
	5. Figures use Very short tab labels fitting the topic.			
	6. Graphs use same colors and line types for same variable in every figure.			
	7. Sensitivity functions. How to plot. Why useful. Notes. Use same colors.			
	8. Ontology consistent in notation of .mod, Figures and Notes and Par sets			
	9. Notation consistent with diagrams in .mod text and on the Website			
	10.Parameters sets: Description and rationale for each			
	11. Loops: purposes and settings; par set			
	12. Optimization re data or other model: descrip, par set, Notes			
Group 3. Verification methods: See STANDARDS-VERIF for detail				
	1. Under Notes: Check off list for the model file verification (X re 10in Gp 3)			
	2. List variables computed in the MML code that are serving as checks			
	3. Commentary on checks or missing checks			
	4. Numerical Methods chosen and why. In notes.			
	5. Solution times chosen; delta t chosen; comments			
Group 4. Validation methods: See STANDARDS-VALID for detail				
	1. Justify initial and boundary conditions in accord with physiology			
	2 .List Data provided and fitted by model, and sources.			
	3. Show fits of data in Figures, and optimization results			
	4. Notes defining contents of each situation, figure or par set			
	5. Parameters estimated and evaluated against literature or other			
Group 5. Uncertainty Quantification: See STANDARDS-UQ for detail				
	1. Parameters and Variables chosen			
	2. Define Measures of uncertainty			
	3. Plots or contour maps of projected results			
Group 6: Scientific Publication: See STANDARDS-PUB for detail				
	1. Summary of the science			
	2. References to subsequent publications or alternative models			
	3. Website for public dissemination, commentary and responses			
	Revised15.07.28 by JBB			

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	STANDARDS 3: The CODE: formatting, annotating	Auth	2nd	Note
Group 1. Basic requirements				
	Code clearly written			
	ALL terms expressed using standard nomenclature			
	Ontology used, and if so consistent?			
	Sections demarcated (Parameters, variables, Cs, BCs, Equations			
	Modular arrangements of code			
	Comments on every line?			
	Comments on every line?			
	Algorithms explained and referenced if needed			
	Short and long descriptions precise and concise			
	References listed			
	Authors, revisors, date and sign contributions			
	References for all parameter values			
	Descriptions and references for subsidiary models			
	Models and graphs all run			
Group 2. Conservation, Balances, that are appropriate to the model				
	Unitary Balance: (units on all variables and parameters)			
	Mass balance: (list constituents whose conservation is checked)			
	Charge balance: (ion currents, membrane potential)			
	Osmotic balance: (volume, total activities, fluxes)			
	Thermodynamic Balance (Haldane constraints on reactions, etc)			
Group 3. Verification: math of model and solution methods are sound				
	Verification checklist complete?			
	Limitation spelled out? Solvers OK?			
	Range of Independence of step size in space or time			
Group 4: Summary of Validation: model is physiologically realistic				
	Data provided, and fitted by model			
	Initial and boundary conditions in accord with physiology			
	Parameters justified (sources provided) and evaluated			
	Model is predictive, shown to fit other data not used as basis			
Group 5: Provision of Source Code and Forum for critiques				
	Website source from which to download model code and data			
	Website or email to accept queries			
	Website for public commentary and responses			
	References to subsequent publications or alternative models			
Group 6. Provenance: Antecedents, derivations and dependencies				
	Peer-reviewed publication (pdf copy)			
	Lineage of the model (list of antecedent models)			
	List higher level models using of which this is a component			
	Shortcomings			
	Future Needs			
	Rev by JBB 15.07.28			

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	STANDARDS.4. VERIFICATION:	Auth	2nd	Note
Group 1: Conservation, Balances		x		
	Unitary Balance: (units on all variables and parameters		xy	
	Mass balance: (list constituents whose conservation is checked)			xyz
	Other balances: Charge, Osmotic , Thermodynamics.			
Group 2.Verification Steps. Checking Math and Numerics of Model				
	All terms defined			
	Numerical Solutions check analytic. Why Methods chosen. In notes.			
	Analytic solutions built into code?			
	Equation formats in similar styles, aligned for easy checking			
	Dependence on time step defined for particular parameter values			
	Dependence on space step defined for particular parameter values			
	Optimizer and loop parameters provided			
	Different solvers gives same results for ODEs			
	Different solvers gives same results for PDEs			
	Implicit eqns solved by iteration? Calculation done how?			
	Commentary on checks or missing checks			
	Solution times chosen; delta t chosen; comments			
	List variables computed in the MML code that are serving as checks			
Group 3: Verification in Data analysis				
	Data available, described and adequate as test			
	Data units matched by model			
	Multiple data sets available			
	Behavioral analysis: Can cover a wide range of situations?			
	Sensitivity analysis defined for conditions that fit data			
Group 4. Validation methods: See STANDARDS-VALID for detail				
	1. Justify initial and boundary conditions in accord with physiology			
	2. List Data provided and fitted by model, and sources.			
	3. Show fits of data in Figures, and optimization results			
	4. Notes defining contents of each situation, figure or par set			
	5. Parameters estimated and evaluated against literature or other			
Group 5. Uncertainty Quantification: See STANDARDS-UQ for detail				
	1. Parameters and Variables chosen			
	2. Define Measures of uncertainty			
	3. Plots or contour maps of projected results			
	4. Methods verified for full range of Monte Carlo ranges used			
Group 6: Scientific Publication: See STANDARDS-PUB for detail				
	1. Summary of verification tests in publication?			
	2. Any failures in verification			
	3. Website for public dissemination of verification methods or tests			

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	STANDARDS.5: VALIDATION TESTING:	Auth	2nd	Note
Group 1: Identification and Description				
	Model Name and No: short and long descriptions complete			
	Code verified and runs correctly. See STANDARDS.4VERIF			
	Diagrams represent the key elements of the system			
	Reference to Publication describing the model			
	Context and Purpose of model defined			
Group 2. Data for Validation testing. FIGURES and NOTES describe validation				
	Experimental data available, and described. Reproducible?			
	The data are defined, figures and parameter sets (All matched)			
	Data figures: Titles appropriate			
	Data figures: axes labeled with symbol, name and units			
	Figures use very short tab labels fitting topic.			
	Graphs use same colors and line types for same variable in every figure.			
	Ontology consistent in notation of .mod, Figures and Notes and Par sets			
	Notation consistent with diagrams, code, Website, publication			
	Parameters sets: Description and rationale for each set of data			
	Optimization re data or other model: Opt Choice, par set, Notes			
	Loops: purposes and settings; par set			
Group 3. Validation evaluation:				
	Initial and boundary conditions in accord with physiology?			
	List Data provided and fitted by model, and sources.			
	Balance checks. (Mass, charge, osmotic, energy)			
	RMS error and CV for all data sets. Different data sets comparable?			
	Show fits of data in Figures, and optimization results			
	Notes defining contents of each situation, figure or par set			
	Parameters estimated and evaluated against literature or other			
	Parameter correlations not near 1			
	Parameters omitted from optimization?			
	Sensitivity functions. How to plot. Why useful. Notes. Use same colors.			
	Residuals random or systematic?			
Group 4. Uncertainty Quantification: See STANDARDS-UQ for detail				
	1. Parameters and Variables chosen re sensitivities to critical parameters			
	2. Define measures of uncertainty for system overall behavior			
	3. Make choices for contour maps and pdfs of projected results			
Group 5: Scientific Publication: See STANDARDS-PUB for detail				
	Summary of the Validation criteria and success			
	Weaknesses in validation; parameters/model components undefined			
	Define future expts, model revisions, commentary and responses			

	STANDARDS.6. UNCERTAINTY QUANTIFICATION:	Auth	2nd	Note
Group 1: Identification of UQ in data, model, computation, parameters				
	Model Name and No:			
	Code verified, runs correctly. See STANDARDS.4VERIF			
	Diagrams for UQ evaluation?			
	Reference to UQ approaches and methods			
	Methods chosen here			
Group 2. DATA UNCERTAINTY: UQ dependence on data				
	Experimental data reproducible?			
	Correlation structure in data sets			
	Description of data, noise, shapes of pdfs			
	Critical missing data that would constrain solutions			
	Constraints from literature. Relevance (species, age, sex, etc)			
Group 3. INPUT and ENVIRONMENT UNCERTAINTY				
	Variability in ICs, Input functions and in assumptions about exper. conditions			
Group 4. PARAMETER UNCERTAINTY:				
	Sensitivity functions. How to plot. Why useful. Notes. Use same colors.			
	Joint sensitivities for partially correlated parameters			
	Loops: stepped setting to illustrate behavior			
	Optimization re data: Confidence, descrip, Correl in covariance matrix			
	Parameters sets: Description and rationale for each param set, Notes			
	Parameters chosen for MonteCarlo. Sensitivities, lit data, constraints			
	Magnitudes of effects on systems behaviors (function space)			
	Ranges and shapes of param pdfs to use in MonteCarlo;			
	Ranges and shapes of cross section through output trajectories			
	Selection of region of predicted responses to characterize			
Group 5. MODEL STRUCTURAL UNCERTAINTY:				
	Modules most subject to uncertainty			
	Modules insensitive for the particular data sets			
	Modules most critical to the need to predict a chosen outcome			
	Notes defining contents of each situation, figure or par set			
	Relation between parameter and model uncertainties			
	Alternative models: Testing by module substitution. Randomized?			
Group 6. Assessing Uncertainty Quantification:				
	Identify major sources of Uncertainty (data, noise, model, params)			
	Meaningfulness and implications of uncertainty			
	Potential means of Reducing Uncertainty			
Group 7: Scientific Publication: See STANDARDS.7.PUB for detail				
	UQ as a major goal of the scientific evaluation			
	Meaning of observed UQs			
	Recommendations re data, models, improving prediction			

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	STANDARDS.7.PUBLICATION	Auth	2nd	Note
Group 1: Identification, Description, and role of MODEL in the field				
	Purpose: to present REPRODUCIBLE SCIENCE with this advancement			
	What is the special contribution of the model			
	Was model used in experiment design? Analysis? Validation? UQ?			
	Context for this work in the field. The science advanced.			
	Novel or confirmatory?			
	Acknowledgments. Authorship criteria.			
Group 2: Technical aspects of the paper				
	Abstract, Intro, Methods, Results, Discussion, Acknowledgment, Appendices			
	Every figure has axes labeled with symbol, name, units. Clean. No clutter			
	Graphs use same colors and line types for same variable in every figure.			
	Ontology consistent in notation of .mod, Figures, Notes, Par sets, Website			
	Equations complete and match notation			
	Parameter and Variable notation: symbol, name, units, description			
	Tables of all parameters, initial conditions, steady state or equilibrium condn			
	Parameter influences: Loops: purposes and settings; par set FIGURES?			
	Optimization re data or other model: description, par set, Notes			
	Graphs; confidence limits, data symbols consistent			
	OPEN SOURCE site identified (DATA, MODEL in Project file)			
	Parameter files and notes for each Figure in the paper? Tested by running?			
Group 3. The Modeling and the analyses				
	Model completely defined, with rationale, provenance,			
	Verification methods: See STANDARDS-VERIF for detail			
	Validation methods: See STANDARDS-VALID for detail			
	Assessment of validation process and adequacy of data and analysis			
	Model variants defined, invalidated, or not invalidated (=working hypoth)			
	Comparing with past work: the novelty (doubts and confidence level)			
	Uncertainty Quantification: See STANDARDS-UQ for detail.			
	Were predictions testable?			
	Reproducibility of Modeling and Data analysis			
	Discussion of contribution to science			
	Future needs defined?			
Group 4. Scientific Publication				
	Journal choice, OPEN SOURCE, freely downloadable			
	Site for Supplements, data, code, project files,			
	The REP, REPRODUCIBLE EXCHANGE PACKAGE, and the storage site			
	Website for public dissemination, commentary and responses			
NOTE	Checklists to be checked by Author and 2 checkers			

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