**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](http://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 | Check1 | 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 |  |  |  |
|  | 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 |  |  |  |

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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 | |  | |  | |  |

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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 | |  |  |  |

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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 give same results for ODEs |  |  |  |
|  | Different solvers give same results for PDEs |  |  |  |
|  | Implicit equations 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 |  |  |  |

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | | 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 fns and assumptions about expt. 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 parameter 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 hypothesis) |  |  |  |
|  | 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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