Microbial-ENzyme Decomposition (MEND) Model
MANUAL

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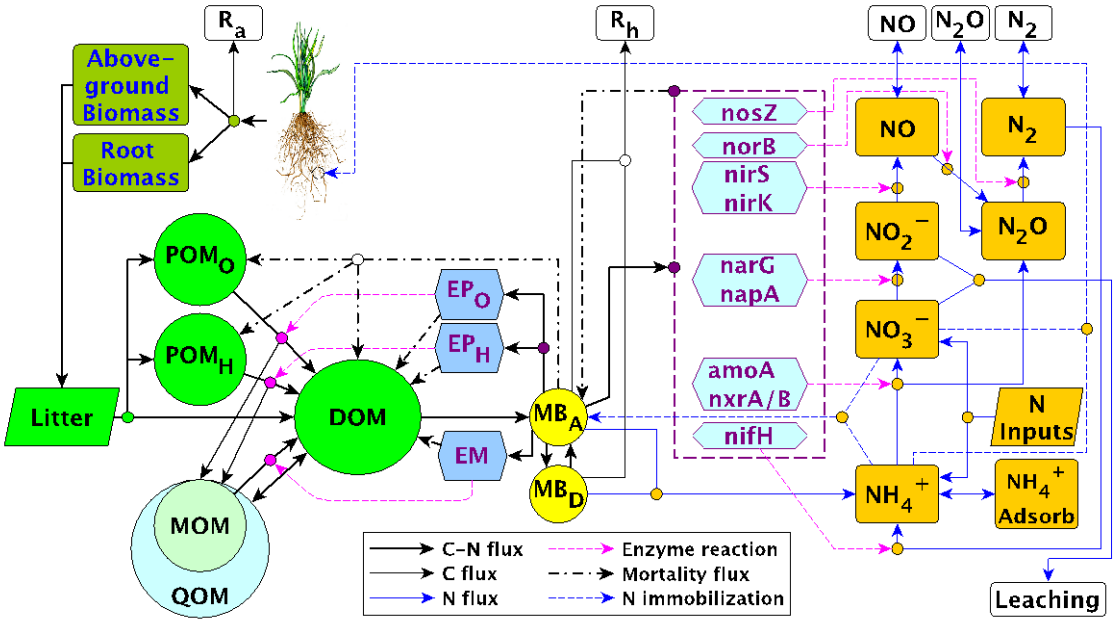


Figure 1 Diagram of the C-N coupled Microbial-ENzyme Decomposition (MEND) model

R_a and **R_h** are autotrophic and heterotrophic respiration, respectively. **POM_O** and **POM_H** are particulate organic matter (**POM**) decomposed by oxidative (**EP_O**) and hydrolytic enzymes (**EP_H**), respectively. **MOM** is mineral-associated OM, which is decomposed by a mixed enzyme group **EM**. Dissolved OM (**DOM**) interacts with the active layer of MOM (**QOM**) through sorption and desorption. **Litter** enters **POM_O**, **POM_H**, and **DOM**. Microbes consist of active (**MB_A**) and dormant microbes (**MB_D**). DOM can be assimilated by **MB_A**. Mineral N deposition and fertilization enter **NH_4^+** and **NO_3^-** that can be immobilized by microbes and taken up by plant roots. NH_4^+ adsorption is also considered. N fixation, nitrification and denitrification are mediated by nitrogenase (**nifH**), ammonia oxidases (**amoA**, **nxrA/B**) and N-reductases (**narG/napA**, **nirS/nirK**, **norB**, **nosZ**), respectively. Mineral N loss pathways include leaching (NO_3^- and NO_2^-) and gas emission (NO, N_2O, and N_2) from soil to atmosphere.

References (#First Authors; *Corresponding Authors):

Jian S, Li J*, **Wang G***, Kluber LA, Schadt CW, Liang J, Mayes MA, 2020. Multi-year incubation experiments boost confidence in model projections of long-term soil carbon dynamics. ***Nature Communications***, 11, 5864.

Gao Q#, **Wang G#**, Yang Y*, Xue K, Xie J, Yu H, Bai S, Liu F, He Z, Ning D, Hobbie SE, Reich PB, Zhou J*, 2020. Stimulation of soil respiration by elevated CO_2 is enhanced under nitrogen limitation in a decade-long grassland study. ***Proceedings of the National Academy of Sciences*** 117, 33317-33324.

Guo X#, Gao Q#, Yuan M#, **Wang G#**, Zhou X, Feng J, Shi Z, Hale L, Wu L, Zhou A, Tian R, Liu F, Wu B, Chen L, Jung CG, Niu S, Li D, Xu X, Jiang L, Escalas A, Wu L, He Z, Van Nostrand JD, Ning D, Liu X, Yang Y, Schuur EAG, Konstantinidis KT, Cole JR, Penton CR, Luo Y, Tiedje JM, Zhou J*, 2020. Gene-informed decomposition model predicts lower soil carbon loss due to persistent microbial adaptation to warming. ***Nature communications*** 11, 4897.

Huang W, Wang K, Ye C, Hockaday WC, **Wang G***, Hall SJ*, 2021. High carbon losses from oxygen-limited soils challenge biogeochemical theory and model assumptions. ***Global Change Biology***. https://dx.doi.org/10.1111/gcb.15867.

Wang G*, Li W, Wang K, Huang W (2021) Uncertainty quantification of the soil moisture response functions for microbial dormancy and resuscitation. ***Soil Biology and Biochemistry*** 160: 108337.

Wang G#*, Huang W#, Mayes MA, Liu X, Zhang D, Zhang Q, Han T, Zhou G*, 2019. Soil moisture drives microbial controls on carbon decomposition in two subtropical forests. ***Soil Biology and Biochemistry*** 130, 185-194.

Wang G*, Jagadamma S, Mayes MA, Schadt CW, Steinweg JM, Gu L, Post WM, 2015. Microbial dormancy improves development and experimental validation of ecosystem model. ***The ISME Journal*** 9, 226-237. doi:10.1038/ismej.2014.120.

Wang G*, Post WM & Mayes MA, 2013. Development of microbial-enzyme-mediated decomposition model parameters through steady-state and dynamic analyses. ***Ecological Applications*** 23, 255-272. doi: 10.1890/12-0681.1.

1 Table of Contents

1 Model Repositories

Model Version	Notes
MEND	Carbon-Nitrogen coupled version: **sINI%Carbon_only = .FALSE.** https://github.com/wanggangsheng/MEND.git
MEND_mult	Multiple-Case Version of MEND: run multiple cases in one-run https://github.com/wanggangsheng/MEND_mult

2 Directories

ID	Directory	Notes
0	model dir	Control Files: **MEND_namelist.nml**
1	src	Source code
2	Userio/inp	Input data **MEND_mult**: includes sub-folder for each case
3	Userio/out	Output data **MEND_mult**: includes sub-folder for each case

3 Major Subroutine Calls

3.1 MEND & MENDcn

0	1	2	3	4
MEND_main	MENDIN			
	SCE	fMEND_OBJ	Par: sINI%LCI0	
			Par: sINI%r0	
			subMEND_INI	subMEND_Files_Open subMEND_CPOOL_UPDATE1 subMEND_NPOOL_UPDATE1 subMEND_CN_UPDATE0
			subMEND_RUN	subMEND_PAR subMEND subMEND_output_rate subMEND_output sOUT_OPT_h sOUT_Day2Mon Extract data for comparison/calibration

3.2 MEND_mult

0	1	2	3	4
MEND_main	MENDIN			
	SCEUA	fMEND_OBJ	Par: sINI%LCI0	
			Par: sINI%r0	
			DO iCase=1,nCase	
			MENDIN_CASE	
			subMEND_INI	
			subMEND_RUN	subMEND_PAR
				subMEND
				subMEND_output_rate subMEND_output
				sOUT_OPT_h
				sOUT_Day2Mon
			END DO	

- '**SIM_obs.out**' combines all '*_SIM_obs.out' for all cases into 1 output file.
- After each MEND run, the total objective function (**fMEND_OBJ**) for multiple cases is calculated by reading data in this file.
- MEND_mult allows different calibration-variables used in various cases. e.g., case1 with 2 variables (CO2 & MBC), case2 with 2 variables (CO2 & DOC). Under this condition, the total OBJ (**fMEND_OBJ**) will include 3 single objectives (CO2, MBC, & DOC).
- 'MEND_namelist.nml' Cali_OBJ_Weight(·) defines OBJ weighting factors for these objectives combined from multiple cases; whereas the OBJ weighting factors for each case ('case.ini' Line 48-57) are NOT used for calibration/optimization.
- MEND_mult runs much slower than MEND. Because MEND_mult REPEATEDLY reads input data for each case (subroutine 'MENDIN_CASE') during each model run. However, MEND only read input data ONCE for a single case.

4 Source Code Files & Major Functions & Subroutines

ID	F90 file	Notes	Major Functions & Subroutines
1	MEND_main	Main program	
2.1	MEND_IN	Control file	○ **MENDIN(sSCE,sINI)**
2.2	*MENDIN_CASE*	*Input data for each case MEND_mult only*	
3	MOD_MEND_TYPE	Data structure for MEND	
4	MOD_MEND	MEND model; Depends on ▪ MOD_MEND_TYPE ▪ MOD_USRFS	○ **subMEND**: MEND model ○ **subMEND_PAR**: MEND parameters modified by temperature, moisture, etc. ○ **subMEND_RUN**: run model continuously with multiple time-steps ○ **subMEND_INI**: model initialization ○ **fMEND_OBJ**: objective function for model evaluation & optimization ○ **sINP_Read**: read input, soil temp & moisture ○ **subMEND_Files_Open**: open output files ○ **subMEND_Files_close**: close output files ○ **sOUT_OPT_VAR_Extract**: extract HOURLY outputs for response variables used for optimization ○ **subMEND_output**: HOURLY outputs for all state variables & fluxes ○ **sOUT_tscale:** convert HOURLY outputs (subMEND_output) to DAILY, MONTHLY & YEARLY outputs ○ **sOUT_ALL_tscale**: convert HOURLY outputs (subMEND_output) to DAILY, MONTHLY & YEARLY outputs, called by sOUT_tscale ○ **sSOBOL_VAR_OBJ**: calculate obj for Sobol sensitivity analysis ○ **sSOBOL_VAR_Read**: Read _VAR_day.out to calculate Sobol obj
5	MOD_OPT_TYPE	Data structure for model optimization	
6	MOD_OPT	Optimization algorithm	○ SCE Depends on ▪ MOD_OPT_TYPE ▪ MOD_MEND
7	MOD_STRING	String utility	○ **StrCompress()**
8	MOD_USRFS	User Functions and Subroutines	
9	MOD_MCMC	MCMC algorithm	

5 Control & Output files

ID	FILE	Notes
	CONTROL FILE:	
1	MEND_namelist.nml	(1) MEND CONTROL file, stored in the model root dir ○ iModel = '0'-run MEND model with parameter sets 'Pinitial'; '1'-model calibration/optimization '2'- uncertainty quantification (UQ) using COFI method, output COFIpar.out '3'-generate objective function values for Sobol Sensitivity analysis '4'-UQ using MCMC '5'-UQ with COFI, output both COFIpar.out & COFIvar.out (see Table 7) '6'-find unfinished parameter sets in previous run (iModel = 3) ○ sSite: site name (2) MEND_mult CONTROL file ▪ Line 11-14: define multiple cases, case names are dir names in inp & out
2	**.ini	CONTROL/INITIAL file for each case, in inp/casedir
	INITIAL FILE:	
1	SOIL_INI.dat	Initialization of SOC pools, stored in 'userio/inp'
	OUTPUT FILES:	**MEND_mult**: Outputs of optimization for all-case are saved in out; Outputs for each case are saved in the out/casedir
1	*_SIM_obs.out	Outputs for SIM vs. OBS for those specific days with OBS. VAR: corresponds to VARid in 'MEND_namelist.nml'. Note: The 'best' parameter set among those 'best' from multiple opt-runs is shown at the last line of this file. You may copy this line to 'MEND_namelist.nml' for future run.
2	* SIM_day.out	Continuous daily SIM results for those variables used for calibration
3	* SIM_mon.out	Continuous monthly SIM results for those variables used for calibration
4	* VAR_hour.out	All state variables: hourly
5	* VAR_day.out	All state variables: daily
6	* VAR_mon.out	All state variables: monthly
7	* VAR_year.out	All state variables: yearly
8	* FLX_hour.out	All fluxes: hourly
9	* FLX_day.out	All fluxes:daily
10	* FLX_mon.out	All fluxes: monthly
11	* FLX_year.out	All fluxes: yearly
12	* ITW_hour.dat	External input (litter), T, SWC, SWP: hourly
13	* ITW_day.dat	External input (litter), T, SWC, SWP: daily
14	* ITW_mon.dat	External input (litter), T, SWC, SWP: monthly
15	* RATE_hour.out	Derived rates: hourly, e.g., active fraction
16	* RATE_day.out	Derived rates: daily
17	* RATE_mon.out	Derived rates: monthly
18	* RATE_year.out	Derived rates: yearly
19	* PAR_hour.out	Parameters modified by T, SWP, pH, etc: hourly
20	* PAR_day.out	Parameters modified by T, SWP, pH, etc: daily
21	* PAR_mon.out	Parameters modified by T, SWP, pH, etc: monthly
22	* PAR_year.out	Parameters modified by T, SWP, pH, etc: yearly
23	* OPT_end.out	'best' parameter sets from multiple independent optimizations
24	* OPT_ini.out	Initial parameters for optimization, log file for any MEND run
25	* OPT_all.out	All parameter sets during optimization, used for COFI UQ
26	* Ndep_hour.out	Mineral N input: hourly

6 Derived Rates: *_*RATE*_hour.out

Col	Name	Units	Notes
1	Hour		Hourly time-step
2	kPOC1	h^{-1}	Equivalent 1st-order decomposition rate; k=VP1*EP1/(POC1 + KP1)
3	kPOC2	h^{-1}	Equivalent 1st-order decomposition rate; k=VP2*EP2/(POC2+ KP2)
4	kMOC	h^{-1}	Equivalent 1st-order decomposition rate; k=VM*EM/(MOC+ KM)
5	kDOC	h^{-1}	Equivalent 1st-order turnover rate; k=[(Vg+Vmt)/Yg]*MBa/(DOC + KD)
6	kMBa	h^{-1}	Equivalent 1st-order turnover rate; k=[(Vg+Vmt)*(1/Yg−1)]*phi + rMORT + pEP+ pEM) * Vmt
7	kMBa_in	h^{-1}	Equivalent 1st-order microbial uptake rate, k=[(Vg+Vmt)/Yg]*phi + Resuscitation/MBa
8	kMBd	h^{-1}	Output rate of dormant microbes, k=(Resuscitation+Maintenance)/MBCd
9	kMBd_in	h^{-1}	Input rate for dormant microbes, k=Dormancy/MBCd
10	kMB	h^{-1}	Turnover rate of total MBC, k=(CO2_gm+ENZ_prod+Mortality)/MBC
11	kMB_in	h^{-1}	Assimilation rate of total MBC, k=uptake/MBC
12	Phi	–	DOC saturation level, = DOC/(DOC + KD)
13	Active_Fraction	–	Fraction of active microbes
14	CUE	–	Apparent carbon use efficiency = [uptake - CO2_gmo]/uptake
15	NUE	–	Apparent nitrogen use efficiency = $[CN_{MB} - CN_{MB\_min}]/(CN_{MB\_max} - CN_{MB\_min})$
16	Balance_Error	mg C g^{-1} soil or mg C cm^{-3} soil	Error for balance check, RE=(TOCend − TOCbeg) − (TOCinp − TOCout)*dt
17	TOCbeg	mg C g^{-1} soil mg C cm^{-3} soil	Total organic carbon at the beginning of the time-step
18	TOCend	Same as above	Total organic carbon at the end of the time-step
19	TOCinp	Same as above	TOC input during the time-step
20	TOCout	Same as above	TOC output during the time-step
21	STP	°C	Soil temperature
22	SWC	$cm^3\ cm^{-3}$	Soil water content
23	SWP	MPa	Soil water potential
24	pH	–	Soil pH

7 SOIL_INI.dat: Model Initialization

nrow= 26

Depth: cm; SOC/POC/MOC/MBC: mgC/cm^3

ID	Property	Value	Notes
1	Depth	10	Soil depth (cm)
2	Sand	0.259	Sand fraction
3	Clay	0.509	Clay fraction
4	CN_MB_mean	8	Mean CN ratio of microbial biomass
5	CN_MB_min	2	Min CN ratio of microbial biomass
6	CN_MB_max	14	Max CN ratio of microbial biomass
7	CN_EP1	3	CN ratio of oxidative enzymes
8	CN_EP2	3	CN ratio of hydrolytic enzymes
9	CN_EM	3	CN ratio of MOM enzymes
10	fQOM	0.01	Fraction of QOM in MOM
11	SOC	21.14	Actually NOT used for modeling
12	POC	5.67	POC1 + POC2
13	MOC	15.47	Mineral-associated Organic Carbon
14	DOC	0.31	Dissolved Organic Carbon
15	MBC	0.53	Default value = 2-5% SOC
16	EP1	0.0011	Default value = 0.005% SOC
17	EP2	0.0011	Default value = 0.005% SOC
18	EM	0.0014	Default value = 0.005% SOC
19	CN_SOM	13	CN ratio of SOM
20	CN_POM	26	CN ratio of Particulate Organic Matter (POM), will be calculated by model
21	CN_MOM	10	CN ratio of MOM, CN_MB < CN_MOM <CN_SOM
22	CN_DOM	10	CN ratio of DOM, default = CN_MOM
23	CN_MB	5.5	CN ratio of microbial biomass
24	NH4	0.003	
25	NO3	0.01	
26	rCN_LIG2LAB	2	See Table 19 rCN = CN_Lignin/CN_Labile in plant litter

8 Input Data

Note: all input data will be converted to hourly rate; see input data format in dir: userio/inp (**MEND_mult**: see casedir in inp)

Input Data	Notes/Sample data	Time scale
Litter input	1) Continuous input, e.g., litter fall, 'MEND_namelist.nml' Type-1 Input Soil depth (cm) in SOIL_INI.dat will be used to convert mg C cm^{-2} $hour^{-1}$ to mg C cm^{-3} $hour^{-1}$	Monthly, daily, or hourly units: mg C cm^{-2} d^{-1} or mg C cm^{-2} $month^{-1}$ or mg C cm^{-2} $hour^{-1}$
	2) Other constant input, e.g., only annual amount available, 'MEND_namelist.nml' Type-2 Input	Convert annual amount to hourly rate
	3) Other constant input during a specific period, e.g., dead roots, 'MEND_namelist.nml' Type-3 Input	Specify total amount & the period (beginning & ending dates)
Soil temperature	'MEND_namelist.nml' preferred units: °C STP.dat	Hourly, daily, or monthly
Soil moisture	'MEND_namelist.nml' preferred units: % will be converted to soil water potential (MPa) using the retention curve parameters given in soil retention curve See 'fSWC2SWP' in 'MOD_MEND.F90' SWC.dat	Hourly, daily, or monthly
Mineral N input	NH4dep.dat; NO3dep.dat	Monthly
C:N ratios	1) Input C:N, see 'MEND_namelist.nml' 2) SOM C:N, see SOIL_INI.dat	

9 Uncertainty Quantification (UQ) by Critical Objective Function Index (COFI): Inputs & Outputs

(1) MEND

iModel = 5

Category	File Name	Notes
Input File	COFIpar.dat	Copy 'out/OPT_all.out' to 'inp/COFIpar.dat', add "OBJ_critical= J_{cr} $J_{\min}$" to 1st line, where $J_{\min}$ denote the optimial/minimum OBJ; and J_{cr} denotes the critical OBJ for UQ: $J_{cr} = J_{opt} \cdot \eta = J_{opt} \cdot \left(1 + \frac{p}{n-p} F_{\alpha,p,n-p}\right)$ J_{opt} is the optimum (min) OBJ, n is the number of OBS, p is the number of PARs, and $F_{\alpha,p,n-p}$ is the value of the F-distribution for α, p, and $n-p$.
Output Files	COFIpar.out	Save parameters that result in $J_{\min}$ <= fObj <= J_{cr}
	COFIvar.out	Save variables on those observational time steps predicted by the PARs in 'COFIpar.out'

(1) MEND_mult

- enabled/corrected on 10/4/2020

MOD_MEND.F90

REAL(8) function fMEND_OBJ(xx, sPAR, sINI, sOUT)

~Line 363–366:

```
if (sINI%iModel.eq.3) then
   write(format101, *) "(", k, "E15.3)"
   write(sINI%iFout_UQvar, format101)dOBS_SIM(:,2)
end if
```

ATTENTION:

- MEND.ini

  iModel = 1; iprint = 1 !! during optimization

  iModel = 3 !! for COFI

- input file: inp/COFIpar.dat

10 sINI%iScenario

Scenario design: data used to conduct scenario analysis beyond calibration period
See 'MEND_namelist.nml' siScenario

iScenario	Notes
1	Repeatedly use 1-yr mean hourly data derived from observed data
2	Repeatedly use multiple-year hourly (observed) data

11 Scenario Design

Parameters controlling the changes in Temperature, Water content & Litterfall Input; specifically, for the subtropical Dinghushan case study, may not be applied to other case studies
See 'MEND_namelist.nml' Scenario design

Parameter	Note
STP_delta	Gradually annual change in Temperature, °C/a
SWC_logis(3)	$$\frac{\theta(t)}{\theta(t_0)} = \frac{p}{1-(1-p)\cdot e^{-r(t-t_0)}}$$ Soil Water Content (SWC, θ) parameters in logistic equation; SWC DECREASES with time (1) $p \in (0,1)$: lower bound for the ratio of $\frac{\theta(t\to\infty)}{\theta(t_0)}$ (2) r > 0: steepness; r = 0 means no changes (3) t_0: reference year
SIN_logis(4)	$$\frac{L(t)}{L_{max}} = \frac{1}{1+\exp\left[\beta_0-\beta_1\cdot(t-t_0)\right]}$$ Litterfall input parameters in logistic equation; Litterfall INCREASES with time (1) $\beta_0 > 0$: intercept (2) $\beta_1 > 0$: steepness; $\beta_1 = 0$ means no changes (3) t_0: reference year (4) fDOC_delta (NOT included in the logistic equation): gradually annual change of DOC fraction in SOC input

12 sINI%iKenetics

Decomposition Kinetics for POC/MOC

See 'MEND_namelist.nml' siKinetics (**MEND_mult**: Line22-23)

iKinetics	Mic-Enz	Kinetics	Equation	Sample MEND_namelist.nml
0	Both	• Michaelis-Menten • MOM decomposition • No MOM-QOM interaction	$F_{dec} = \frac{V_M \cdot E \cdot S}{K_M + S}$	MEND_Enz-Mic.ini
1	No Enz	First Order	$F_{dec} = k_M \cdot S$	MEND_No-Enz.ini
2	Both	Second Order	$F_{dec} = k_M \cdot E \cdot S$	
10	Mic-Enz	• Michaelis-Menten • QOM decomposition • MOM-QOM interaction	$F_{dec} = \frac{V_M \cdot E \cdot S}{K_M + S}$	
11	None	First Order	$F_{dec} = k_M \cdot S$	MEND_No-Enz-Mic.ini

13 sINI%iHR

Calculation Method for Growth & Maintenance Respiration from Active Microbes

iHR	Method	Notes
0	$HR_g = \max\left[D, \left(\frac{1}{Y_G} - 1\right)\frac{V_g \cdot BA \cdot D}{K_D + D}\right]$ $HR_m = \max\left[D, \left(\frac{1}{Y_G} - 1\right)\frac{V_m \cdot BA \cdot D}{K_D + D}\right]$	HR_g or HR_m is constrained by DOC
1	$HR_{gm} = \max\left[D, \frac{1}{Y_G} \times \frac{(V_g + V_m) \cdot BA \cdot D}{K_D + D}\right] \times (1 - Y_g)$ $HR_g = HR_{gm} \times \frac{V_g}{V_g + V_m}, HR_m = HR_{gm} \times \frac{V_m}{V_g + V_m}$	Total microbial uptake is constrained by DOC, HR_g or HR_m is a fraction of total uptake

14 sINI%iTmp_Func

Temperature Response Function

iTmp_Func	fT	Notes
0	fTArh: Arrhenius Equation	See function in MOD_MEND
1	fTQ10: Q10 method	See function in MOD_MEND

15 sINI%iError

Error code during model runs

sINI%iError	Description

< 0	Mass balance error
	function fMEND_OBJ(xx, sPAR, sINI, sOUT):
	sINI%rOBJ = dabs(const_FillValue)
	fMEND_OBJ = dabs(const_FillValue)
	
	SUBROUTINE sSOBOL_VAR_OBJ():
	if(itype.eq.0) then
	dSIM_t0 = dabs(const_FillValue)
	else
	Sobol_obj = dabs(const_FillValue)
	end if

-11	Error in 1st carbon balance check
-12	Error in 1st nitrogen balance check
-21	Error in 2nd carbon balance check
-22	Error in 2nd nitrogen balance check

16 MEND State Variables (C & N Pools)

ID	Soil C and/or N pool	Pool Name	Variable name
1	Particulate organic matter (POM) decomposed by oxidative enzymes	POM_O	C pool: *PO*; N pool: *PON*
2	POM decomposed by hydrolytic enzymes	POM_H	*PH*; *PHN*
3	Mineral-associated organic matter	MOM	*M*; *MN*
4	Dissolved organic matter	DOM	*D*; *DN*
5	Active MOM interacting with DOM	QOM	*Q*; *QN*
6	Active microbial biomass	MB_A	*BA*; *BAN*
7	Dormant microbial biomass	MB_D	*BD*; *BDN*
8	Oxidative enzymes decomposing POM_O	EP_O	*EPO*; *EPON*
9	Hydrolytic enzymes decomposing POM_H	EP_H	*EPH*; *EPHN*
10	Enzymes decomposing MOM	EM	*EM*; *EMN*
11	Ammonium oxidase	ENH4	*ENH4*; *ENH4N*
12	Nitrate reductase	ENO3	*ENO3*; *ENO3N*
13	Nitrite reductase	ENO2	*ENO2*; *ENO2N*
14	Nitric oxide reductase	ENO	*ENO*; *ENON*
15	Nitrous oxide reductase	EN2O	*EN2O*; *EN2ON*
16	Nitrogenase	EN2	*EN2*; *EN2N*
17	Adsorbed ammonium	NH_4^+ Adsorb	*NH4ads*
18	Ammonium	NH_4^+	*NH4*
19	Nitrate	NO_3^-	*NO3*
20	Nitrite	NO_2^-	*NO2*
21	Nitric oxide	NO	*NO*
22	Nitrous oxide	N_2O	*N2O*
23	Dinitrogen	N_2	*N2*

17 MEND Parameters

17.1 MEND Parameters

('MEND_namelist.nml' INITIAL PARAMETERS) (**MEND_mult**: Line 28-57)

ID	Parameter	Description	Range	Units	Eq#
1	LF_0	Initial fraction of PO, $LF_0 = PO/(PO+PH)$	(0.1, 1.0)	—	
2	r_0	Initial active fraction of microbes, $r_0 = BA/(BA+BD)$	(0.01, 1)	—	
3	fR_a	Scaling factor for autotrophic respiration (R_a)	(0.1, 0.4)	—	11
4	$fINP$	Scaling factor for litter input rate	(0.1, 0.9)	—	1
5	Vd	Maximum specific decomposition rate $Vd_{PO} = Vd_{PH} = Vd_M = Vd$	(0.1, 100)	mg C mg^{-1} C h^{-1}	24–26
6	K_{PO}	Half-saturation constant (HSC) for PO decomposition	(40,100)	mg C cm^{-3} soil	24
7	fK_M	$K_M = K_{PO} \times fK_M$, $K_{PH} = K_{PO}/fK_M$ K_{PH} and K_M are HSC for PH and M, respectively	(2, 20)	—	25–26
8	Q_{max}	Maximum sorption capacity	(0.5, 5.0)	mg C cm^{-3} soil	27
9	K_{ba}	Binding affinity for DOM, sorption rate $k_{ads} = k_{des} \times K_{ba}$	(1, 16)	(mg C cm^{-3} soil)$^{-1}$	27
10	k_{des}	Desorption rate for DOM	(1e-4, 0.01)	mg C cm^{-3} soil h^{-1}	28
11*	r_E	Enzyme turnover rate	(1e-4, 0.01)	mg C mg^{-1} C h^{-1}	39, 41
12*	p_{EP}	$[V_m \times p_{EP}]$ is the production rate of EP (EPO + EPH), V_m is the specific maintenance rate for BA	(1e-4, 0.05)	—	38
13*	fp_{EM}	$fp_{EM} = p_{EM}/p_{EP}$, $[V_{mt} \times p_{EM}]$ is the production rate of EM	(0.1, 5.0)	—	38
14*	f_D	Fraction of decomposed PO and PH allocated to D	(0.05, 1)	—	3
15*	g_D	Fraction of dead BA allocated to D	(0.01, 1)	—	1
16	g_{PO}	$(1 - g_D) \cdot g_{PO}$ is the fraction of dead BA entering PO	(0.05, 0.2)	—	2
17*	V_g	Maximum specific uptake rate of D for growth	(1e-3, 0.1)	mg C mg^{-1} C h^{-1}	29
18*	α	$= V_m/(V_g + V_m)$, V_m is max specific maintenance rate	(0.01, 0.5)	—	29
19*	K_D	HSC for microbial uptake of D	(1e-4, 0.5)	mg C cm^{-3} soil	29
20*	$Y_g(T_{ref})$	Intrinsic C use efficiency at reference temperature (T_{ref})	(0.1, 0.6)	—	29
21	k_{Yg}	Slope for Y_g dependence of temperature	(1e-3, 0.016)	1/°C	29
22*	Q_{10}	Q_{10} for temperature response function	(1.2, 2.5)	—	
23	γ	Max microbial mortality rate = $V_m \times \gamma$	(0.1, 20)	—	32
24	β	Ratio of dormant maintenance rate to V_m	(5e-4, 0.05)	—	36
25	ψ_{A2D}	Soil water potential (SWP) threshold for microbial dormancy; both ψ_{A2D} & $\psi_{D2A} < 0$	(–0.6, –0.2)	MPa	
26	τ	$\psi_{D2A} = \psi_{A2D} \times \tau$, ψ_{D2A} is the SWP threshold for microbial resuscitation	(0.1, 0.9)	—	
27	ω	Exponential in SWP function for microbial dormancy or resuscitation	(1, 6)	—	
28	$VN_{im,BA}$	Max specific microbial N immobilization rate $VN_{im,NH4} = VN_{im,BA} \cdot NH4/(NH4 + NO3)$ $VN_{im,NO3} = VN_{im,BA} \cdot NO3/(NH4 + NO3)$	(1e-4, 0.1)	mg N mg^{-1} C h^{-1}	48, 49
29	KSN_{BA1}	HSC for microbial immobilization of NH_4^+	(1e-4, 0.01)	mg N cm^{-3} soil	48–50
30	KSN_{BA2}	HSC for microbial immobilization of NO_3^-	(1e-4, 0.01)	mg N cm^{-3} soil	48–50
31*	VN_{nit}	Max specific nitrification rate (VN_1)	(0.1, 1000)	mg N mg^{-1} C h^{-1}	42
32*	VN_{denit}	Max specific denitrification rate, $VN_j = VN_{denit}$, j=2–5	(1e-5, 0.1)	mg N mg^{-1} C h^{-1}	44
33*	VN_{fix}	Max specific N fixation rate (VN_6)	(1e-4, 0.1)	mg N mg^{-1} C h^{-1}	45
34	KSN_1	HSC for nitrification	(1e-4, 0.1)	mg N cm^{-3} soil	42
35	KSN_2	HSC for denitrification of NO_3^- and NO_2^- (KSN_3)	(1e-4, 0.1)	mg N cm^{-3} soil	44
36	KSN_4	HSC for denitrification of NO and N_2O (KSN_5)	(1e-4, 0.1)	mg N cm^{-3} soil	44
37	KSN_6	HSC for N fixation	(1e-4, 0.1)	mg N cm^{-3} soil	45
38*	VN_{VG}	Max plant N uptake rate; $VN_{VG,NH4} = VN_{VG,NO3} = VN_{VG}$	(1e-6, 1e-3)	mg N cm^{-3} h^{-1}	51, 52
39	KSN_{VG1}	HSC for plant uptake of NH_4^+	(1e-4, 0.01)	mg N cm^{-3} soil	51
40	KSN_{VG2}	HSC for plant uptake of NO_3^-	(1e-4, 0.01)	mg N cm^{-3} soil	52
41	ω_{VG}	Exponential for calculating $rGPP$ as a function of GPP	(0.01, 1)	—	52
42*	$NH4_{max}$	Maximum sorption capacity for NH_4^+	(1e-5, 0.01)	mg N cm^{-3} soil	53
43	$K_{ba,NH4}$	Binding affinity for NH_4^+	(1, 1e4)	(mg N cm^{-3} soil)$^{-1}$	53
44	r_{leach}	Scaling factor for NO_3^- and NO_2^- leaching	(0.01, 1)	—	54

Note1: ‘MEND_namelist.nml’ Cali_Calibrate (**MEND_mult**: Line 31-57), Column ‘Calibrate’: ‘1’ means the parameter will be calibrated, ‘0’ mean no-calibration.
Note2: ‘MEND_namelist.nml’ Pintital (**MEND_mult**: Line 61), initial parameter values, will override the values in Column ‘Initial’ at Line 78-104.

17.2 MEND Parameters that may be pre-determined

Parameter	Regression Equation	R^2	p-value
K_{P1} (mg C g^{-1} soil): half-saturation constant for POC decomposition	$K_{P1} = 41.58 \times DOC + 44.95$ $K_{P1} = 0.62 \times (\%Sand) + 45.56$ $K_{P1} = 1.07 \times POC + 50.13$	0.97 0.82 0.64	0.01 0.10 0.20
K_M (mg C g^{-1} soil): half-saturation constant for MOC decomposition	$K_M = 455.11 \times DOC + 400.42$ $K_M = 4.13 \times MOC + 425.75$	0.98 0.73	0.01 0.15
K_D (mg C g^{-1} soil): half-saturation constant for microbial uptake of DOC	$K_D = 0.33 \times MBC + 0.21$	0.63	0.21
Q_{max} (mg C g^{-1} soil): maximum sorption capacity	$Q_{max} = 0.012 \times MOC + 3.43$ $Q_{max} = 0.011 \times SOC + 3.39$	0.98 0.91	0.01 0.04
K_{ba} ([mg C g^{-1} soil] $^{-1}$): binding affinity	$K_{ba} = -0.082 \times (\%Sand) + 11.23$	0.84	0.08
K_{des} (mg C g^{-1} soil h^{-1}): desorption rate	$K_{des} = -0.0059 \times DOC + 0.0059$	0.95	0.02
$V_{death} = V_{mt} \times gamma$: microbial death rate	[Hansen, 1990, DAISY] 0.001 – 0.01 d^{-1}, 4×10^{-5} – 4×10^{-4} h^{-1}		
Vd	We can also roughly determine Vd by a few model trials. (1) Try to fix the value of Vd and calibrate other parameters to fit Rh observations. If the goodness-of-fit of Rh is good (i.e., R^2 >0.4) and the PBIAS of Rh is good (i.e., $\lvert PBIAS \rvert = \left\lvert \frac{\bar{Y}_{sim} - \bar{Y}_{obs}}{\bar{Y}_{obs}} \right\rvert$ <10%), we would conclude the simulated enzyme activities ($EA = Vd \cdot EC$) or decomposition rates ($FR = (Vd \cdot EC)/(K + S) = EA/(K + S)$) are good. (2) Check the simulated total SOM-degrading enzyme concentrations (*EC: variable name ENZD_C in* xxx_VAR_xxx.out). Total		

	enzyme concentrations should have the magnitude of 0.1–1% of MBC. (3) If EC values are too high, increase the value of Vd, do model calibration again, we would see a decrease in EC.		
fR_a :Scaling factor for autotrophic respiration (R_a)	As $Ra = fRa * GPP$, we could calculate the fRa directly use lm(Ra~GPP+0), i.e., $$fR_a = \frac{\overline{R_a}}{\overline{GPP}}$$		
fINP: scaling factor for litter input rate	we can roughly determine fINP, particularly for the control treatment, which is often assumed to be at quasi steady state, i.e., average input rate to SOC = mean heterotrophic respiration rate. Thus $$fINP = \frac{\overline{R_h}}{\overline{GPP}}$$ Regarding the fINP for other treatments, we may use the same fINP as the control treatment or adjust it carefully. Basically, fINP should NOT be calibrated simultaneously with other parameters. If we need to calibrate fINP, we have to set a narrow parameter range for fINP based on our knowledge.		
fD, gD	I prefer NOT to calibrate fD and gD if we could fix them (e.g., fD=0.75, gD=0.50) to achieve good model performance. However, we may need to calibrate fD and gD to obtain good results.		
rE, pEP, fpEM	usually I will calibrate these three parameters: rE, pEP, fpEM.		
Yg and kYg	avoid calibrating Yg(Tref) and kYg simultaneously. We need to fix one of them and calibrate the other one. If we want to fix kYg, try default		

	value 0.01 first. If we want to fix Yg(Tref), try default value 0.3 first.		
Q10	check namelist file: siTmp_Func = 0: Arrhenius Equation, siTmp_Func = 1: Q10 Equation is used.		
γ	try to fix it by default value $\gamma = 0.1$ first.		

Notes:
SOC: soil organic carbon; POC: particulate organic carbon; MOC: mineral-associated organic carbon; DOC: dissolved organic carbon; MBC: microbial organic carbon. Units: mg C g^{-1} soil.
%Sand: percentage of sand in soil.

18 Response Variables for Model Calibration/Optimization

18.1 Calibration Variables in MEND_namelist.nml

Note: 'MEND_namelist.nml' CALIBRATION DATA; see data format in dir: userio/inp
MEND_mult: Line 45-57 in '*.ini' in 'userio/inp/casedir'

Column	Column Name	Notes
1	VARid	Variable ID
2	VAR	Variable Name
3	Units	Units
4	Calibrate	'1'-data available for calibration, '0'-unavailable
5	tstep	Time-step: 0-hourly, 1-daily, 2-monthly, **5**-mean_value_of_last2years, **6**-mean_value_of_last_80%data. Usually the observations are regarded as data measured during an hourly-scale, the simulation results will be averaged during 1 day (24-h) to compare with the observations
6	Obs_file	File with observation data if available
7	Obs_file_column	Column id for the data, currently not used
8	OBJ	Type of objective function (minimization): ▪ NSEC: Nash-Sutcliffe Efficiency Coefficient (Coefficient of Determination), see 'f1NSE' in 'MOD_USRFS.F90' ▪ MARE: Mean Absolute Relative Error, see 'fMARE' in 'MOD_USRFS.F90' ▪ CORR: correlation coefficient, see 'f1CORR' ▪ CORl: CORR with log10-tranformed data, see 'f1CORR' ▪ MARt: MARE with tolerance, see 'fMARE_tolerance' ▪ NSEn: NSEC for normalized data, see 'f1NSE_norm' ▪ MARn: MARE for normalized data, see 'fMARE_norm' ▪ AVGr: |ratio – AVGsim/AVGobs|, see 'f1RAVG_ratio'
9	OBJ_Weight	Weighting factor for each OBJ, will be normalized in the code

Microbial biomass carbon (MBC) should be included in model calibration. If we don't have MBC measurements. Assume MBC = 2-5% SOC, which is used for both initial MBC and reference value for simulated MBC. As for model calibration:

Cali_tstep: 5 (mean MBC of last 2 years) or 6 (mean MBC of last 80% data)

Cali_OBJ: 'MARt'

Cali_OBJ_Tolerance: 0.1 or 0.05 (mean MBC within 10% or 5% of the reference MBC)

18.2 Add a new Calibration Variable

(1) MEND_namelist.nml (see Section 16): add a new variable, e.g., No.41 for rMBA (active fraction of microbes)

Cali_varid(41:44) = 41, 42, 43, 44

```
   Cali_VAR(41:44)          = 'rMBA',          'TBD1',          'TBD2',          'TBD3'
   Cali_Units(41:44)        = 'NONE',          'mgN-cm3-h',     'mgN-cm3-h',     'mgN-
cm3-h'
   Cali_Calibrate(41:44)    =  0,              0,               0,               0
   Cali_tstep(41:44)        =  2,              2,               2,               2
   Cali_obs_file(41:44)     = 'rMBA.obs',      'EA_NO2.obs',    'EA_NO.obs',
'EA_N2O.obs'
   Cali_obs_file_column(41:44) =  2,           2,               2,               2
   Cali_OBJ(41:44)          = 'MARE',          'MARE',          'MARE',
'MARE'
   Cali_OBJ_Weight(41:44)   =  2,              2,               2,               2
   Cali_OBJ_Tolerance(41:44)  =  0,            0,               0,               0
```

(2) MOD_MEND_TYPE.f90

```
INTEGER, PARAMETER:: const_nVAR0     = 44          !# of variables for calibration
```

(3) MOD_MEND.F90

```
SUBROUTINE sOUT_OPT_h(nVAR,nHour,iHour,dSIM,sPAR,sOUT,VARopt_int)
```

```
case (41)   !!Active fraction of microbes
    dSIM(iHour,j) = sOUT%CPOOL%MBA/max(sOUT%CPOOL%MB,1d-6)

    or

    SUBROUTINE
    sOUT_OPT_VAR_Extract(nVAR,nHour,iHour,dSIM,sPAR,sOUT,VARopt_int)
```

(4) Prepare observed data file for rMBA: rMBA.obs

19 Parameter Optimization Algorithm

Note: '**MEND_namelist.nml**' SCE parameters, (**MEND_mult**: Line 16-20)
only 3 parameter '**nrun**' , '**iniflg**' and '**iprint**' are required to edit

Parameter	Notes
nrun	# of runs for optimization, these opt-runs are independent of each other. There is a different random seed for each opt-run. nrun <= 200
iniflg	flag on whether to include the initial point (Line 108) in population = 0, not included = 1, included
iprint	Flag on whether to print all points generated during optimization = 0, no printing =1, print to *_OPT_all.out for COFI UQ analysis

20 sINI%VAROpt_int

sINI%VAROpt_int(sINI%nVAROpt, 3)

Column1: i	Column2: n	Column3: t: tstep
Index of calibrated output VARiable	# of observations	0(hourly) 1(daily) 2(monthly) 3(seasonal): to_do 4(yearly) 5(mean, last 2 years) 6(mean, last 80% period)

21 CN Ratios in 3 Litter Pools

3 litter pools: Lignin, Cellulose, and Labile
Assume their fractions in Carbon mass = f_Lig, f_Cel, f_Lab
f_Lig + f_Cel + f_Lab = 1
Assume CN_Cel = 500
Assume CN_Lig/CN_Lab = rCN
Assume overall CN in litter pool = CN
N mass balance:

$$N = \frac{C}{CN} = \frac{C \cdot f_{Lig}}{CN_{Lab} \cdot rCN} + \frac{C \cdot f_{Cel}}{CN_{Cel}} + \frac{C \cdot f_{Lab}}{CN_{Lab}}$$

thus

$$CN_{Lab} = \left[\frac{f_{Lig}}{rCN} + f_{Lab}\right] \Big/ \left[\frac{1}{CN} - \frac{f_{Cel}}{CN_{Cel}}\right]$$

$$CN_{Lig} = CN_{Lab} \times rCN$$

22 MEND (non-MPI) Configuration/Compiling on OSX & Cygwin/Unix

22.1 Dependency of source code

- Edit 'nbproject/**Configurations.xml**' to define dependency of source code for compilation, e.g.,

MOD_MEND depends on 2 modules (MOD_MEND_TYPE & MOD_USRFS);
MOD_OPT depends on 3 modules (MOD_OPT_TYPE, MOD_MEND, & MOD_USRFS).

- See './**Configurations.xml**' for example:

```
<item path="src/MEND_IN.F90" ex="false" tool="2" flavor2="0">
 <fortranCompilerTool>
  <additionalDep>${OBJECTDIR}/src/MOD_STRING.o ${OBJECTDIR}/src/MOD_USRFS.o
${OBJECTDIR}/src/MOD_MEND_TYPE.o ${OBJECTDIR}/src/MOD_MEND.o
${OBJECTDIR}/src/MOD_OPT_TYPE.o</additionalDep>
 </fortranCompilerTool>
</item>
<item path="src/MEND_main.F90" ex="false" tool="2" flavor2="0">
 <fortranCompilerTool>
  <additionalDep>${OBJECTDIR}/src/MOD_USRFS.o ${OBJECTDIR}/src/MOD_MEND_TYPE.o
${OBJECTDIR}/src/MOD_MEND.o ${OBJECTDIR}/src/MOD_OPT_TYPE.o
${OBJECTDIR}/src/MOD_OPT.o ${OBJECTDIR}/src/MOD_MCMC.o</additionalDep>
 </fortranCompilerTool>
</item>
<item path="src/MOD_MCMC.F90" ex="false" tool="2" flavor2="0">
 <fortranCompilerTool>
  <additionalDep>${OBJECTDIR}/src/MOD_USRFS.o ${OBJECTDIR}/src/MOD_MEND.o
${OBJECTDIR}/src/MOD_OPT_TYPE.o</additionalDep>
 </fortranCompilerTool>
</item>
<item path="src/MOD_MEND.F90" ex="false" tool="2" flavor2="0">
 <fortranCompilerTool>
  <additionalDep>${OBJECTDIR}/src/MOD_USRFS.o
${OBJECTDIR}/src/MOD_MEND_TYPE.o</additionalDep>
 </fortranCompilerTool>
</item>
<item path="src/MOD_MEND_TYPE.F90" ex="false" tool="2" flavor2="0">
</item>
<item path="src/MOD_OPT.F90" ex="false" tool="2" flavor2="0">
 <fortranCompilerTool>
  <additionalDep>${OBJECTDIR}/src/MOD_USRFS.o ${OBJECTDIR}/src/MOD_MEND.o
${OBJECTDIR}/src/MOD_OPT_TYPE.o</additionalDep>
 </fortranCompilerTool>
</item>    <item path="src/MOD_OPT_TYPE.F90" ex="false" tool="2" flavor2="0">
</item>
<item path="src/MOD_STRING.F90" ex="false" tool="2" flavor2="0">
</item>
<item path="src/MOD_USRFS.F90" ex="false" tool="2" flavor2="0">
</item>
```

22.2 gcc/gfortran Installation

(1) OSX

https://github.com/fxcoudert/gfortran-for-macOS/releases

(2) Windows (install gcc/gfortran/make)
Cygwin, https://www.cygwin.com/
Install package Devel

22.3 gdb Installation on Mac OS Mojave

(1) sudo port install gdb@8.0.1
Note: version after gdb8.0.1 does NOT compatible with High Sierra
(2) ln -sf /opt/local/bin/ggdb /usr/local/bin/gdb
(3) create gdb certificate (e.g., gdbcert)
1) Open Applications/Utilities/Keychain Access
2) In menu, open **Keychain Access > Certificate Assistant > Create a Certificate**
3) Give it a name (e.g. `gdbcert`)
Identity type: Self Signed Root
Certificate type: Code Signing
Check: Let Me Override Defaults
4) Continue until "Specify a Location For"
5) Set Keychain location to System. If this yields the following error: `Certificate Error: Unknown Error =-2,147,414,007` Set Location to Login, Unlock System by click on the lock at the top left corner and drag and drop the certificate gdbcert to the System Keychain.
6) Create certificate and close Certificate Assistant.
7) Find the certificate in System keychain.
8) Double click certificate.
9) Expand **Trust**, set **Code signing** to `Always Trust`

(4) Restart taskgated in terminal: sudo killall taskgated
`Another method:`
`ps aux | grep taskgated`
in the terminal to find the PID number of taskgated, and then killed it with
`sudo kill -9 <insert here your PID number>`

(5) (Option) Enable root account:
- Open System Preferences
- Go to User & Groups > Unlock
- Login Options > "Join" (next to Network Account Server)
- Click "Open Directory Utility"
- Go up to **Edit > Enable Root User**

(6) Codesign gdb certificate:
Create a file gdb.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
<!DOCTYPE plist PUBLIC "-//Apple//DTD PLIST 1.0//EN"
"http://www.apple.com/DTDs/PropertyList-1.0.dtd">
<plist version="1.0">
<dict>
    <key>com.apple.security.cs.debugger</key>
    <true/>
```

```
</dict>
</plist>
```

```
sudo codesign --entitlements gdb.xml -fs gdb2 /usr/local/gdb-8.0.1/bin/gdb
```

if this command doesn't print anything, it means the binary is correctly signed.

5/3/2019: gdb works now☺

(7) (Option) Disable root account (see #10)

(8) gdb does NOT work in NetBeans. However, it will work if we run NetBeans with sudo: sudo '/Applications/NetBeans/NetBeans 8.2.app/Contents/Resources/NetBeans/bin/netbeans'
(9) gdb works in command line: sudo gdb ./mend

Problem: gdb stop at a line without breakpoint in MEND_main.F90
Solution: in SourceTree, commit the code changes

22.4 NetBeans Configuration on OSX & Windows

(1) Install NetBeans with JDK

- NetBeans 11.0 (April 30, 2019) (Not Working sometimes)

https://github.com/carljmosca/netbeans-macos-bundle
./install.sh

- NetBeans 8.2 with JDK 8u111 (April 30, 2019) (Working for both OSX and Windows)

https://www.oracle.com/technetwork/java/javase/downloads/jdk-netbeans-jsp-3413139-esa.html
Accept License Agreement
Select file to download

- NetBeans 12.1 (Nov 6, 2020 Working with jdk-{Version <= 13})

```
Failed to install any plugin with jkd-15, e.g., c/c++
```

- Check jdk versions:

```
ls /Library/Java/JavaVirtualMachines
```

- copy and paste pack200, unpack200 and unpack.dil from bin of jdk-{Version <= 13} into the bin of jdk-{Version > 13}.

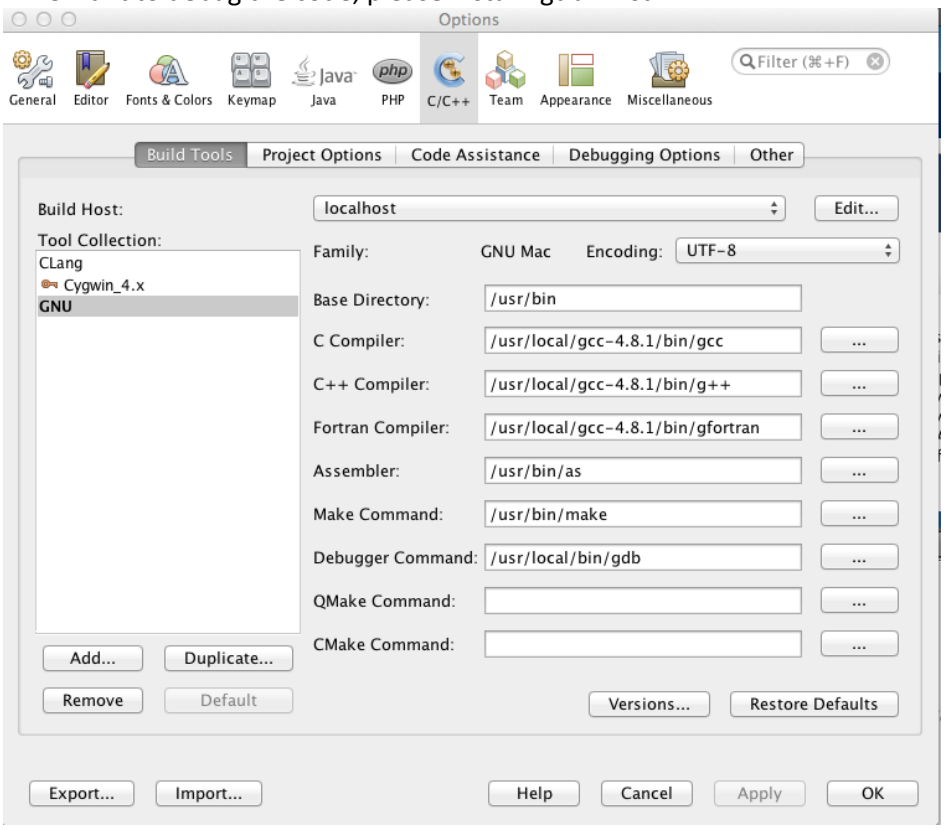
- C/C++ plugin for NetBeans 9.0
  - **Tools > Plugins > Settings** tab **>** click the **Add** button.
  - On the **Update Center Customizer** screen:
    - Enter some value in the **Name** field (e.g. *"My plugins"*),
    - in the **URL** field Enter

    http://updates.netbeans.org/netbeans/updates/8.2/uc/final/distribution/catalog.xml.gz

- Click the **OK** button.
- This should create a new entry in the **Configuration of Update Centers** list in the **Settings** tab.
- Checking that new entry should instantly add plugins to the **Available Plugins** tab.
- Click the **Available Plugins** tab, then click the **Category** column to sort the entries by category.
- The **Name** of the entry at the top of the list should be **C/C++**. If so, you have successfully made the plugin available:

➢ JDK 11
https://www.oracle.com/technetwork/java/javase/downloads/jdk11-downloads-5066655.html

(2) gcc/gfortran Compiler configuration
(i) preference->Options->C/C++->Build Tools
If something is missing (e.g., gfortran), we need to install it first, then click the button "…" to locate the package.
If we want to debug the code, please install "gdb" first.

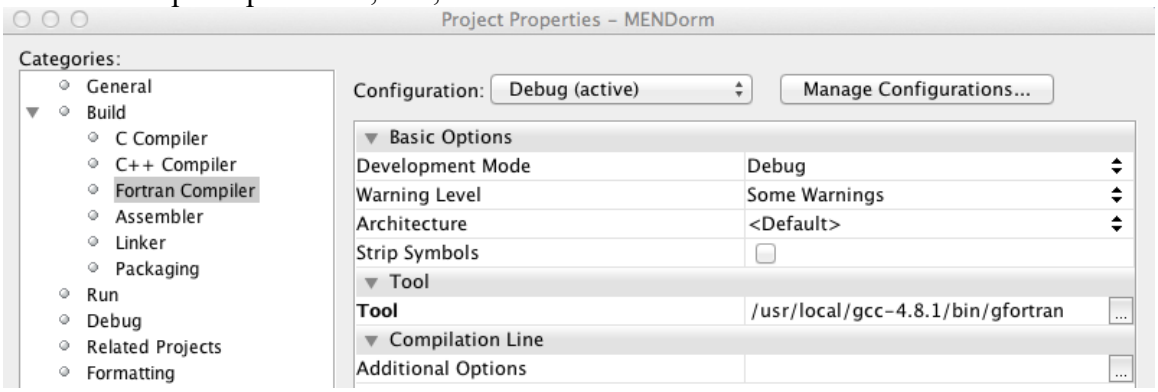


(3) In NetBeans, File -> New Project -> Samples -> C/C++ -> Fortran Hello World Application -> Select the Project Location & Create a Project Name, e.g., "MEND"

(4) A Project Folder will be generated, e.g., "/a1/a2/MEND"
(5) Delete the Sample Source Files "bar.f". & "foo.f"
(6) Copy the following folders & files into "/a1/a2/MEND": src, userio, MEND_namelist.nml
(7) Edit 'nbproject/**Configurations.xml**' to define dependency of source code for compiling (see Section 21.1)
(8) Right click on project name "MEND" in left window, Project Properties->Build->Fortran Compiler->Tool
Specify the absolute path for "gfortran"
Additional Options:
-ffpe-trap=invalid,zero,overflow (check floating point exceptions)
-finit-local-zero (initialize local INTEGER, REAL,and COMPLEX variables to zero, LOGICAL variables to false, and CHARACTER variables to a string of null bytes)

this will modify /Users/wgs/Dropbox_job/Model/MEND/nbproject/Makefile-Debug.mk:

```
# Fortran Compiler Flags
FFLAGS=-ffpe-trap=invalid,zero,overflow -finit-local-zero
```



(9) Compile a single FORTRAN file by right-clicking the file name and click "Compile File (F9)"
(10)Compile all source code files: Right click on project name "MEND", Clean and Build
(11)Run model in NetBeans: click icon
(12)Run model in Terminal:

```
cd  MEND
ln -sf ./dist/Debug/GNU-MacOSX/mend mend
./mend
```

(13)Solution to Error: ld: library not found for -lSystem
Solution 1: xcode-select --install
Solution 2 (11/4/2020: works for new laptop):

```
sudo softwareupdate -l
```

the Command Line Tools were listed as an update, so I installed them using

```
sudo softwareupdate -i -a
```

https://developer.apple.com/download/more/

22.5 Compiling on Unix

(1) Copy the NetBeans configured MEND folder to another system (Windows-Cygwin or Unix)
(2) Edit file "**/nbproject/Makefile-Debug.mk**": replace "**FC=/**/gfortran**" with the full path of "gfortran" on the new machine system, e.g., FC=/usr/local/gcc-8.1/bin/gfortran-8.1

```
# Fortran Compiler Flags
FFLAGS=-ffpe-trap=invalid,zero,overflow -finit-local-zero
```

(3) "cd" into the MEND model directory
(4) make clean
(5) **make -k** : NOT required anymore, as 'nbproject/**Configurations.xml**' defines dependency of source code for compilation
(6) **make**
(7) The "mend" or "**mend.exe**" file will be generated if there are no errors
(8) If the path for "mend.exe" is "/dist/Debug/…/mend.exe", type "**./dist/Debug/…/mend.exe**" to run model
(9) Another option to run model: copy "/dist/Debug/…/mend.exe" to root-dir of MEND model, type "**./mend.exe**"
(10) A 3rd option to run model

```
cd  MEND
ln -sf ./dist/Debug/…/mend.exe mend.exe
./mend.exe
```

##Example: Begin----------

```
## login into cluster 129.15.40.234
ssh your-username@129.15.40.234
## pass: *******

## make a new directory
makdir test

## switch to your local machine
## copy a folder from local machine to remote machine
## enter the local directory containing MEND
scp -r MEND your-username@129.15.40.234:~/test/MEND2

## switch to 129.15.40.234
which gfortran

/usr/bin/gfortran

vi nbproject/Makefile-Debug.mk
## edit the following line
FC=/usr/bin/gfortran
## save and exit

make clean
```

```
    ## build the model, generate excutable file
    make


    ls -lt dist/Debug/GNU-MacOSX/

    ## link the executable file
    ln -sf dist/Debug/GNU-MacOSX/mend mend

    ## run executable file
    ./mend
```
##Example: End----------

22.6 Text Editor

- Sublime Text

https://www.sublimetext.com/

Tools -> Command Palette -> install package control
Tools -> Command Palette -> Package Control: Install Package ->SideBarEnhancements
Tools -> Command Palette -> Package Control: Install Package ->Fortran

Preferences -> Setting
Preferences.sublime-settings – User

```
{
        "color_scheme": "Packages/Color Scheme - Default/Monokai.sublime-color-
scheme",
        "ignored_packages":
        [
                "Vintage"
        ],
        "word_wrap": false
}
```

22.7 Eclipse Configuration for non-MPI MEND

➢ Installing Photran in Eclipse on a Machine With Internet Access

To install Photran, start Eclipse, then...

1. Click on Help > Install New Software...
2. Click on the "Available Software Sites" hyperlink
3. Look for http://download.eclipse.org/tools/ptp/updates/luna in the list.
    1. If it is in the list, check the box next to it (if it is not already checked).
    2. If it is not in the list...
        1. Click on the "Add..." button
        2. In the Location field,
           type http://download.eclipse.org/tools/ptp/updates/luna
        3. Click OK to close the Add Site dialog. This will return you to the Install dialog.
4. Click OK to close the Preferences dialog (i.e., the list of available software sites). This will return you to the Install dialog.
5. In the "Work with:" dropdown, choose http://download.eclipse.org/tools/ptp/updates/luna
6. Expand "Fortran Development Tools (Photran)" and check the box next to "Photran End-User Runtime"
7. If you are running Linux and have the Intel Fortran Compiler installed, or if you are on a Macintosh and have the IBM XL Fortran compiler installed, expand "Fortran Compiler Support" and select the appropriate compiler.
8. Click on the "Next" button
9. If you get an error message, see below for troubleshooting information.
10. Click the Finish button and agree to the license to complete the installation.

- New -> Fortran Project -> Executable (Gnu Fortran on MacOS X) First. Check "Generate Makefiles automatically"
- ***ATTENTION***: Fortran-90 files must have extension of "**f90**", NOT "F90", otherwise resulting in failure to build project in Eclipse
- ***ATTENTION***: module: the Fortran file name must be the same as the module name
- Compile code: After "makefile" and "subdir.mk" are generated, uncheck "Generate Makefiles automatically". Now we can modify "makefile" and "subdir.mk", e.g.,

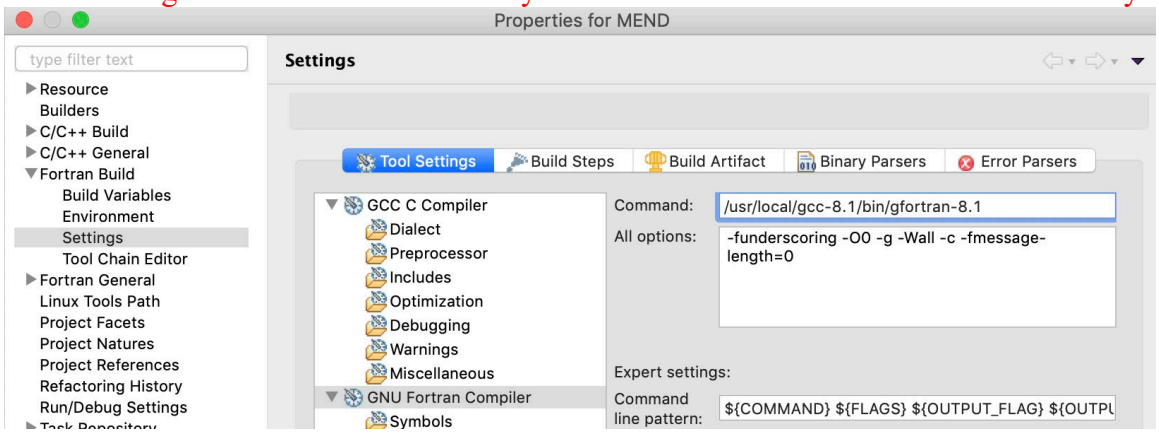
```
FC=/usr/local/gcc-8.1/bin/gfortran-8.1
Then use $(FC)

Clean:
        -$(RM) ./*.mod
```

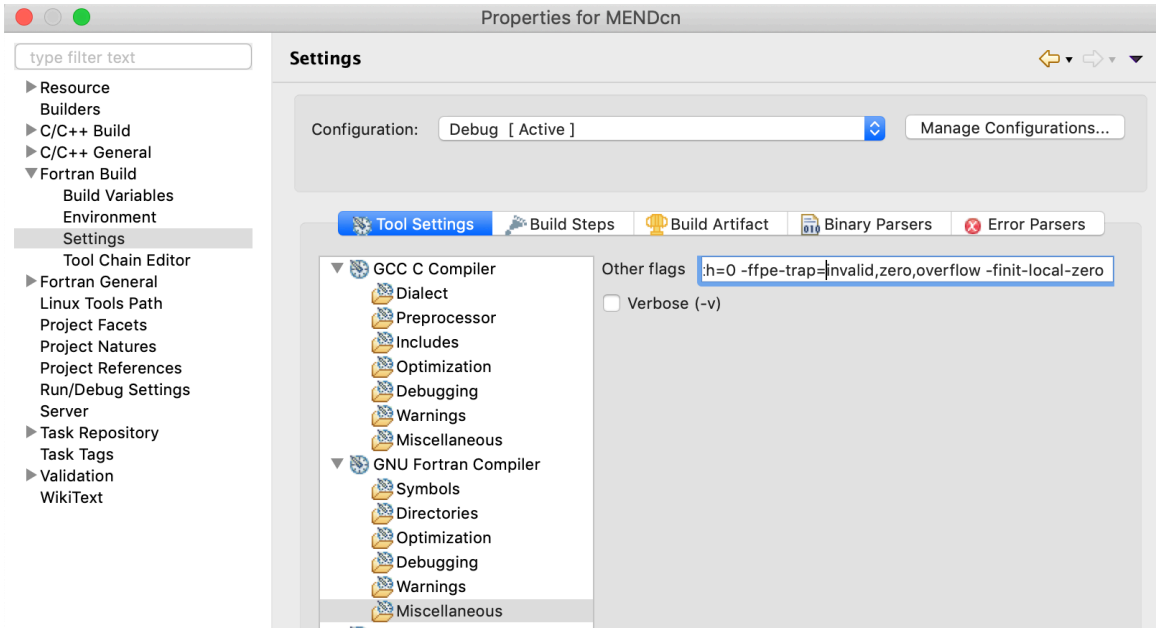
- Debug with gdb

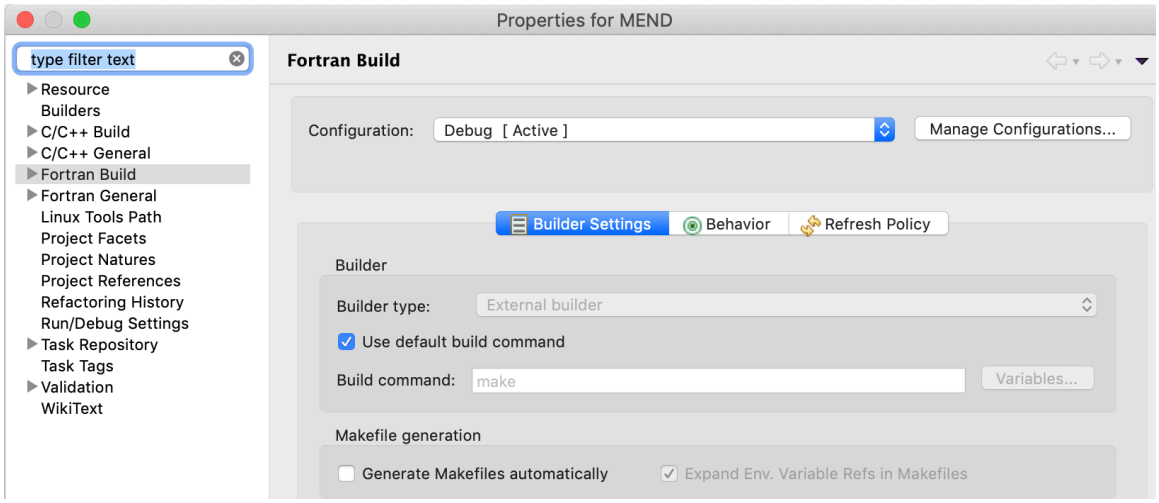
ATTENTION: use full path
/usr/local/gdb8.3.1/bin/gdb
/Users/wgs/.gdbinit

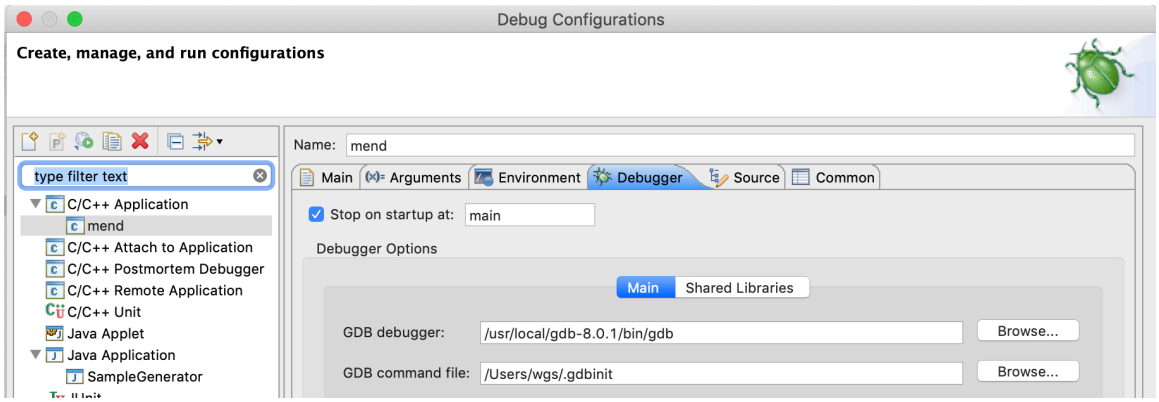
set startup-with-shell off

“Tool Settings” tab will NOT be seen if you uncheck “Generate Makefiles automatically”









23 Tips on unix and git commands

23.1 iTerm2:

https://iterm2.com/

- disable line wrapping:

tput rmam

- enable line wrapping:

tput smam

23.2 git

- .gitignore NOT working correctly

git rm -r --cached .
git add .