Microbial-ENzyme Decomposition (MEND) Model
MANUAL

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References:

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. Model

Model Version	Notes
MEND	C-ONLY; Model development https://wanggangsheng@bitbucket.org/wanggangsheng/mend
MEND_mult	Multiple-Case Version of MEND: run multiple cases in one-run https://wanggangsheng@bitbucket.org/wanggangsheng/mend_mult

2. Directories

ID	Directory	Notes
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

0	1	2	3	4
MEND_main	MENDIN			
	SCEUA	fMEND_OBJ	Par: sINI%LCI0	
			Par: sINI%r0	
			subMEND_INI	
			subMEND_RUN	subMEND_PAR
				subMEND
				subMEND_output_rate subMEND_output
				sOUT_OPT_h
				sOUT_Day2Mon

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.ini' Line 25-26 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	MENDIN	Control file	
2.2	MENDIN_CASE	Input data for each case	
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 ○ sOUT_OPT_h: extract HOURLY outputs for response variables used for optimization ○ sOUT_OPT: convert HOURLY data (sOUT_OPT_h) to DAILY or MONTHLY data ○ subMEND_output: HOURLY outputs for all state variables & fluxes ○ sOUT_tscale: convert HOURLY outputs (subMEND_output) to DAILY & MONTHLY outputs ○ sOUT_ALL_tscale: convert HOURLY outputs (subMEND_output) to DAILY & MONTHLY outputs, called by sOUT_tscale
5	MOD_OPT_TYPE	Data structure for model optimization	
6	MOD_OPT	Optimization algorithm	Depends on ▪ MOD_OPT_TYPE ▪ MOD_MEND
7	MOD_STRING	String utility	
8	MOD_USRFS	User Functions and Subroutines	

5. Control & Output files

ID	FILE	Notes
	CONTROL FILE:	
1	MEND.ini	(1) MEND CONTROL file, stored in the model root dir ○ Line 3-4: iModel = '0'-run MEND model with parameter sets in Line 108; '1'-model calibration/optimization '2'-uncertainty quantification (see Table 7) ○ Line 5-6: site name (2) MEND_mult CONTROL file ▪ Line 11-14: define multiple cases, case names are dir names in inp & out
	**.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.ini', Line 55-64. 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.ini' Line-108 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	*_FLX_hour.out	All fluxes: hourly
8	*_FLX_day.out	All fluxes:daily
9	*_FLX_mon.out	All fluxes: monthly
10	*_ITW_hour.dat	External input (litter), T, SWC, SWP: hourly
11	*_ITW_day.dat	External input (litter), T, SWC, SWP: daily
12	*_ITW_mon.dat	External input (litter), T, SWC, SWP: monthly
13	*_RATE_hour.out	Derived rates: hourly, e.g., active fraction
14	*_RATE_day.out	Derived rates: daily
15	*_RATE_mon.out	Derived rates: monthly
16	*_PAR_hour.out	Parameters modified by T, SWP, pH, etc: hourly
17	*_PAR_day.out	Parameters modified by T, SWP, pH, etc: daily
18	*_PAR_mon.out	Parameters modified by T, SWP, pH, etc: monthly
19	*_OPT_end.out	'best' parameter sets from multiple independent optimizations
20	*_OPT_ini.out	Initial parameters for optimization
21	*_OPT_all.out	All 'good' parameter sets during each loop of optimization

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	Balance_Error	mg C g^{-1} soil mg C cm^{-3} soil	Error for balance check, RE=(TOCend – TOCbeg) – (TOCinp – TOCout)*dt
15	TOCbeg	mg C g^{-1} soil mg C cm^{-3} soil	Total organic carbon at the beginning of the time-step
16	TOCend	mg C g^{-1} soil mg C cm^{-3} soil	Total organic carbon at the end of the time-step
17	TOCinp	mg C g^{-1} soil h^{-1} mg C cm^{-3} soil h^{-1}	TOC input during the time-step
18	TOCout	mg C g^{-1} soil h^{-1} mg C cm^{-3} soil h^{-1}	TOC output during the time-step

7. Uncertainty Quantification (UQ): Inputs & Outputs

iModel = 2

Category	File Name	Notes
Input File	UQpar.dat	Copy '*_OPT_all.out', add "OBJ_critical= J_{cr}" to 1st line, where 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	*_UQpar.out	Save parameters that result in fObj <= J_{cr}
	*_UQvar.out	Save variables on those observational time steps predicted by the PARs in '*_UQpar.out'

8. Decomposition Kinetics for POC/MOC

See 'MEND.ini' Line 72-73 (**MEND_mult**: Line22-23)

sINI%iKenetics	Kinetics	Equation
0	Michaelis-Menten	$F_{dec} = \frac{V_M \cdot E \cdot S}{K_M + S}$
1	First Order	$F_{dec} = k_M \cdot S$
2	Second Order	$F_{dec} = k_M \cdot E \cdot S$

9. 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	Time scale
Litter input	1) Continuous input, e.g., litter fall, 'MEND.ini' Line 33-38	Monthly, daily, or hourly
	2) Other constant input, e.g., only annual amount available, 'MEND.ini' Line 39-40	Convert annual amount to hourly rate
	3) Other constant input during a specific period, e.g., dead roots, 'MEND.ini' Line 41-42	Specify total amount & the period (beginning & ending dates)
Soil temperature	'MEND.ini' Line 23-26 preferred units: °C	Hourly, daily, or monthly
Soil moisture	'MEND.ini' Line 27-32 preferred units: % will be converted to soil water potential (MPa) using the retention curve parameters given in Line 32. See 'fSWC2SWP' in 'MOD_MEND.F90'	Hourly, daily, or monthly

10.MEND Parameters ('MEND.ini' Line 75-104) (MEND_mult: Line 28-57)

ID	Parameter	Description	Apriori range	Units
1	LF_0	Initial fraction of P_1, $LF_0 = P_1/(P_1+P_2)$	(0.1, 1.0)	—
2	r_0	Initial active fraction of microbes, $r_0 = BA/(BA+BD)$	(0.01, 1)	—
3	V_{P1}	Maximum specific decomposition rate for P_1	(10, 100)	mg C mg^{-1} C h^{-1}
4	V_{P2}	Maximum specific decomposition rate for P_2	(10, 100)	mg C mg^{-1} C h^{-1}
5	V_M	Maximum specific decomposition rate for M	(0.05, 20)	mg C mg^{-1} C h^{-1}
6	K_{P1}	Half-saturation constant for P_1 decomposition	(40, 100)	mg C g^{-1} soil
7	K_{P2}	Half-saturation constant for P_2 decomposition	(1, 40)	mg C g^{-1} soil
8	K_M	Half-saturation constant for M decomposition	(100, 1000)	mg C g^{-1} soil
9	Q_{max}	Maximum sorption capacity	(0.5, 5)	mg C g^{-1} soil
10	K_{ba}	Binding affinity	(1, 16)	(mg C g^{-1} soil) $^{-1}$
11	K_{des}	Desorption rate, Sorption rate $K_{ads} = K_{des} \times K_{ba}$	(0.0001, 0.01)	mg C g^{-1} soil h^{-1}
12	r_E	Turnover rate of EP_1, EP_2, and EM	(0.0001, 0.01)	mg C mg^{-1} C h^{-1}
13	p_{EP}	$[V_{mt} \times p_{EP}]$ is the production rate of EP (EP_1 + EP_2), V_{mt} is the specific maintenance rate for active microbes	(0.0001, 0.05)	—
14	fp_{EM}	$fp_{EM} = p_{EM}/p_{EP}$, $[V_{mt} \times p_{EM}]$ is the production rate of EM	(0.5, 2.0)	—
15	f_D	Fraction of decomposed P_1 and P_2 allocated to D	(0.1, 1)	—
16	g_D	Fraction of dead BA allocated to D	(0.1, 1)	—
17	V_g	Maximum specific uptake rate of D for growth	(0.001, 0.05)	mg C mg^{-1} C h^{-1}
18	$alpha$	$= V_{mt} / (V_g + V_{mt})$	(0.05, 0.5)	—
19	K_D	Half-saturation constant for microbial uptake of D	(0.01, 0.5)	mg C g^{-1} soil
20	Y_g	True growth yield	(0.1, 0.64)	—
21	Y_{g_sl}	Slope for Y_G dependence of temperature, see function 'fT_CUE' in 'MOD_MEND.F90'	(0.001,0.016)	1/°C
22	w_{die}	Exponential in SWP function for microbial death, see function 'fSWP_Death' in 'MOD_MEND.F90'	(0.5, 4)	—
23	$gamma$	Max microbial mortality rate = $V_{mt} \times gamma$	(0.1, 20)	—
24	$beta$	Ratio of dormant maintenance rate to V_{mt}	(0.0005,0.05)	—
25	WP_{A2D}	Soil water potential (SWP) threshold for microbial dormancy; note that WP_{A2D} & WP_{D2A} are |SWP|, since SWP <0. See functions 'fSWP_A2D' & 'fSWP_D2A' in 'MOD_MEND.F90'	(0.2, 0.6)	–MPa
26	tau	$WP_{D2A} = WP_{A2D} \times tau$, WP_{D2A} is the SWP threshold for microbial resuscitation	(0.1, 0.8)	—
27	w_{dorm}	Exponential in SWP function for microbial dormancy or resuscitation,	(0.5, 6)	—

Note1: 'MEND.ini' Line 78-104 (**MEND_mult**: Line 31-57), Column 'Calibrate': '1' means the parameter will be calibrated, '0' mean no-calibration.
Note2: 'MEND.ini' Line 108 (**MEND_mult**: Line 61), initial parameter values, will override the values in Column 'Initial' at Line 78-104.

11.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

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.

12.Response Variables for Model Calibration/Optimization

Note: 'MEND.ini' Line 52-64; 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	Available	'1'-data available, '0'-unavailable
5	tstep	Time-step: 0-hourly, 1-daily, 2-monthly. 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: ▪ NSEC: Nash-Sutcliffe Efficiency Coefficient, see 'f1NSE' in 'MOD_USRFS.F90' ▪ MARE: Mean Absolute Relative Error, see 'fMARE' in 'MOD_USRFS.F90'
9	OBJ_Weight	Weighting factor for each OBJ, will be normalized in the code

13.Parameters for the Optimization Algorithm

Note: '**MEND.ini**' Line 66-70, (**MEND_mult**: Line 16-20)
only 2 parameter '**nrun**' and '**iniflg**' 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

14.sINI%VAROpt_int(sINI%nVAROpt, 3)

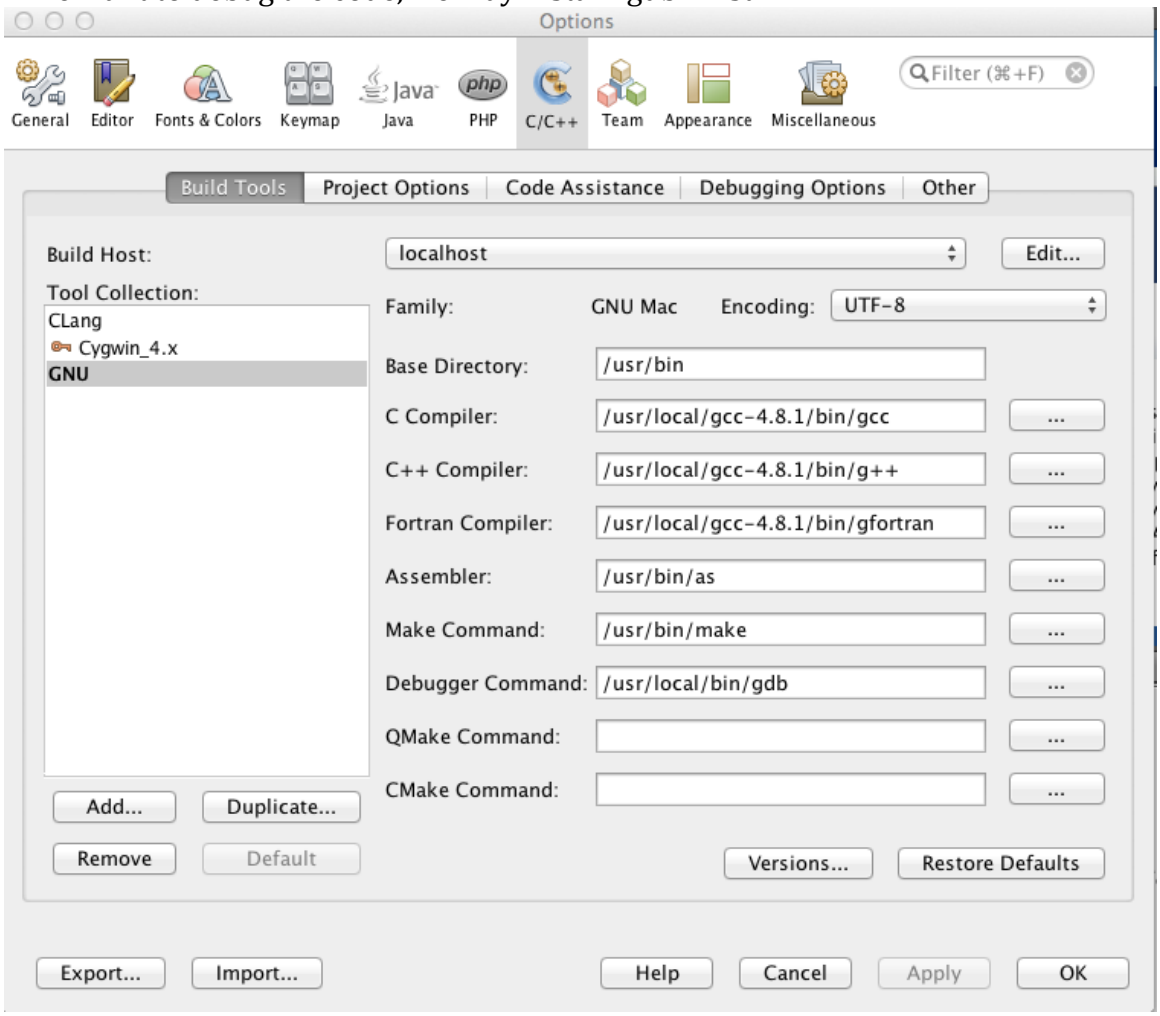
Column1: i	Column2: n	Column3: t
Index of calibrated output VARiable	# of observations	tstep: 0(hourly) 1(daily) 2(monthly) 3(seasonal): to_do 4(yearly) 5(mean)

15.NetBeans Configuration on MAC & Compilation on Cygwin/Unix

15.1 NetBeans Configuration on MAC

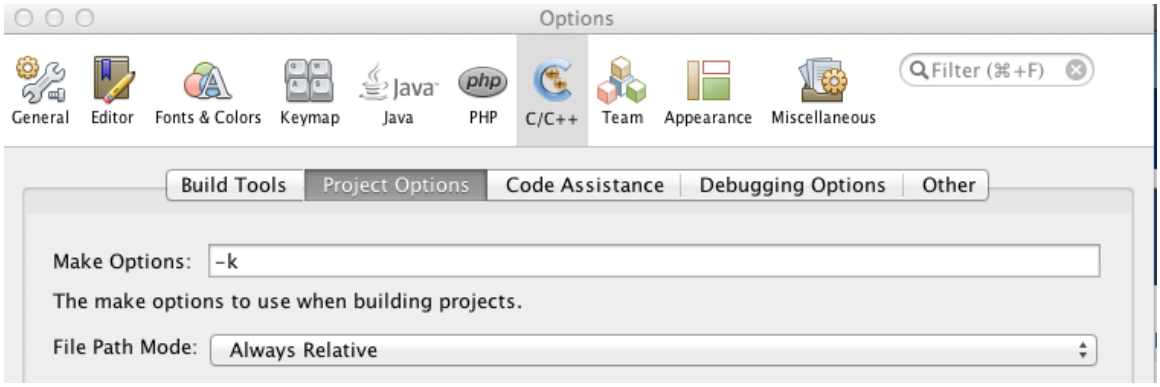
(1) Install NetBeans with JDK
http://www.oracle.com/us/technologies/java/jdk-7-netbeans-download-432126.html

(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, we may install "gdb" first.

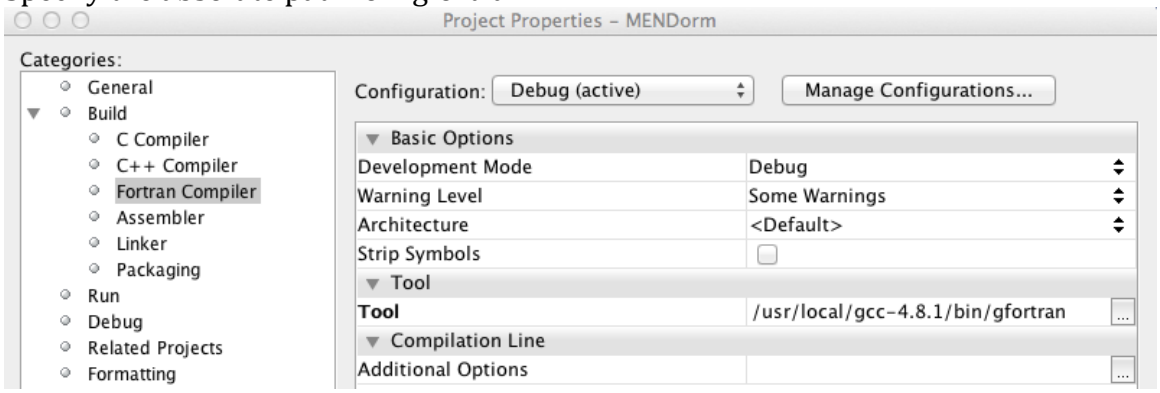


(ii) preference->Options->C/C++->Project Options

- **add "-k" to "Make Options"**: Continue as much as possible after an error. While the target that failed, and those that depend on it, cannot be remade, the other prerequisites of these targets can be processed all the same.
- **With the "-k" option, we don't need to know the compilation orders of multiple modules (one module may depend on other prerequisites). We just implement "build" for multiple times and ignore build errors until it shows "Build Successful".**
- **Take MEND as an example, MOD_MEND depends on 2 modules (MOD_MEND_TYPE & MOD_USRFS); MOD_OPT depends on 3 modules (MOD_OPT_TYPE, MOD_MEND, & MOD_USRFS). We need to "build" 3 times to make it successful. We do NOT need to compile the fortran file one by one.**



(3) Project Properties->Build->Fortran Compiler->Tool
Specify the absolute path for "gfortran"



(4) We can compile a single FORTRAN file by right-clicking the file name and click "Compile File (F9)"

(5) If a module is modified, e.g., a new variable is declared in the module, suggest to "Clean" the project then re-do "build": right-click project name->More Build Commands->Clean Project.

(6) Run model in NetBeans: click icon 

15.2 Compilation on Cygwin/Unix

(7) Copy the NetBeans-configured MEND folder to another system (Windows-Cygwin or Unix)
(8) Edit file "**/nbproject/Makefile-Debug.mk**": replace "**FC=/**/gfortran**" with the full path of "gfortran" on the new machine system
(9) "cd" into the MEND model root-dir
(10) make clean
(11) repeat "**make -k**" for multiple (e.g., n) times (3 times for current MEND model), ignore errors in the first (n-1) times. Actually the modules will be compiled in the first (n-1) compilation.
(12) The "**mendorm.exe**" file will be generated if there's no errors after n times
(13) If the path for "mendorm.exe" is "/dist/Debug/…/mendorm.exe", type "**./dist/Debug/…/mendorm.exe**" to run model
(14) Another option to run model: copy "/dist/Debug/…/mendorm.exe" to root-dir of MEND model, type "**./mendorm.exe**"