Flowcharts

Contents

The *MedeA* environment provides graphical flowcharts to support the efficient construction of complex computational protocols. These flowcharts can be easily created to describe and control the flow of calculations, allowing simple and straightforward access to *MedeA*'s various computation engines, such as LAMMPS, GIBBS, VASP, MOPAC and Gaussian. These different engines may be combined within a single flowchart, so that a VASP optimization of a unit cell, for example, may be employed as a prelude to a larger scale LAMMPS simulation using an embedded atom method forcefield. In addition, the structure can be modified within the flowchart using the provided building and editing capabilities.

The backbone of the flowchart infrastructure is the Tcl language (see https://www.tcl.tk/) which can be directly accessed within custom-scripting stages. Once created the flowcharts can be saved as ASCII files allowing them to be reused and distributed.

Although flowcharts are customizable and flexible their use is straightforward. In this section the basic concepts are summarized, allowing for the construction of both simple and complex flowcharts. Additional details for specific tools are provided elsewhere within the *MedeA* User's Guide.

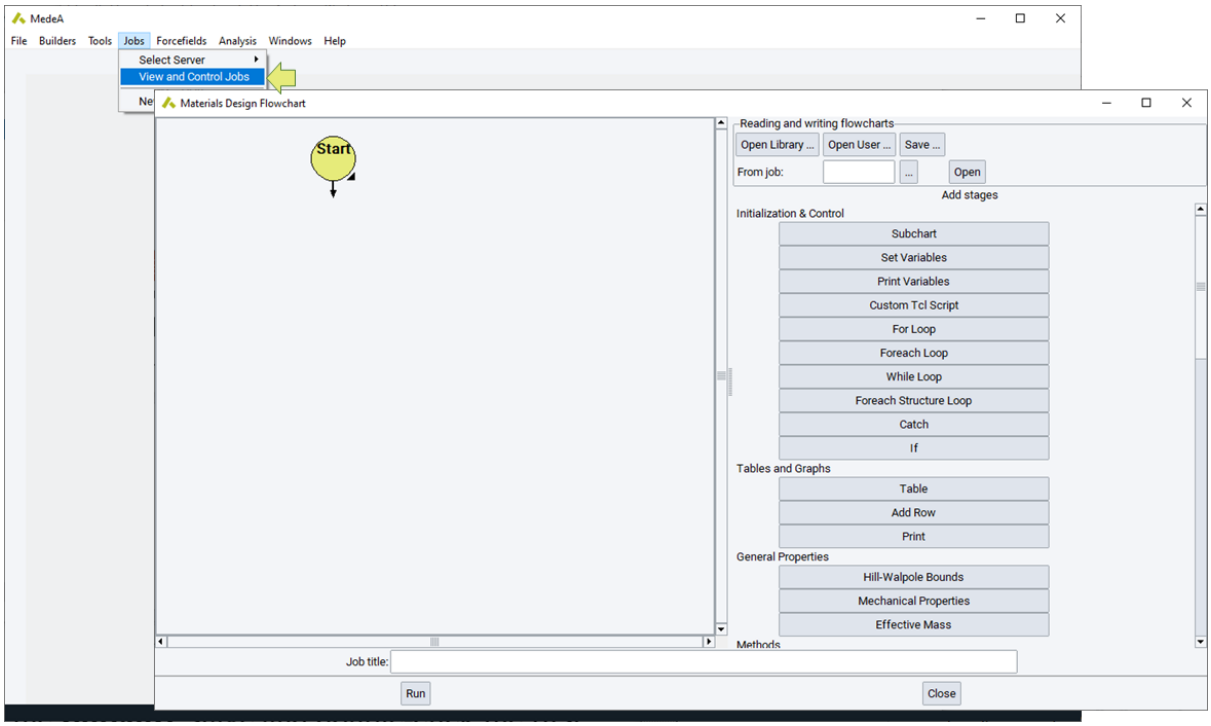
1 Flowcharts Overview

Flowcharts are accessed via the Job Control >> New Job... menu item. This command yields the main flowchart user interface, where flowcharts are constructed, read from disk or from previous calculations, or saved to the disk.

Flowcharts provide a variety of control capabilities, such as a While Loop, For Loop, Foreach Structure Loop, If and Foreach Loop. This allows for considerable flexibility in the automation of simulations. For example, a scan of possible system temperatures and pressures for molecular dynamics calculations may be achieved with nested Foreach loops.

Additionally, custom Tcl scripting may be included in a flowchart. Key results from simulation stages are available as variables, which can be operated on, tabulated, and also used to control subsequent stages,

allowing the convenient construction of highly automated procedures for selected applications. If more complex manipulation of the results are required, a custom Tcl stage can be used to process the outputs of the current and any previous stages.



Materials Design flowcharts begin with the Start command which is automatically placed on the left-hand pane of the flowchart dialog. Typically, after initiating a flowchart with a Start stage, a number of variables will be set using a Set Variables stage. The stage is added to the flowchart by clicking the Set Variables button on the right-hand pane.

In general, stages are added to a flowchart by clicking the appropriate element on the right-hand pane of the flowchart dialog or user interface. Once added to a flowchart, most stages may be edited by either right-clicking that element and selecting Edit, or double-clicking on that stage.

A summary of the functionality and use of specific flowchart elements is provided below.

2 Initialization and Control

This section of the flowchart interface provides the following stages: Start, Subchart, Set Variables, Print Variables, Custom Tcl Script, and loop related commands: For Loop, Foreach Loop, While Loop, Foreach Structure Loop, Catch and If.

As discussed above, every flowchart begins with a Start stage, this is employed as the starting point of execution for the flowchart, and is automatically included in the flowchart. The Subchart stage is simply a container that can hold other flowcharts. This provides a convenient way to break up a large more complicated flowchart into simpler parts and provides a simple way to include a previous flowchart as a building block into a more complicated protocol.

The Set Variables stage allows the user to set the value and units of specific variables that will be employed in later stages in the flowchart. For example, the Set Variables stage can be used to set:

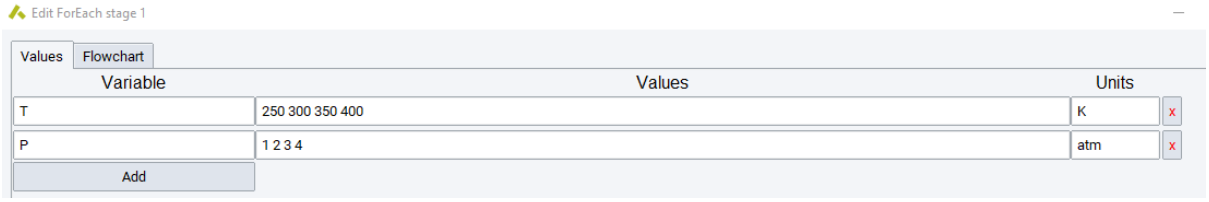
Variable	Value	Units
T	300	K
tstep	1	fs
P	1	atm

These variables will then be used throughout subsequent stages in LAMMPS calculations, which employ `T`, `tstep`, and `P` as default variables for temperature, timestep, and pressure respectively. This centralization of the variable setting is convenient in exploring the effect of the system variables on simulated properties. Once declared variables can be accessed, in accordance to the Tcl paradigm, by adding a `$` sign in front of the variable name, for example, the variable `tstep` can be accessed with `$tstep`.

The Print Variables reports (calculated) variables matching a specific name, including variables created and made accessible by any previous stage. These variables can be printed to tables or added to structure lists.

The Custom Tcl Script allows you to enter, or retrieve from a file Tcl commands (see https://www.tcl.tk/) which may be used to carry out specific actions during the execution of a flowchart. This can be useful in preparing result summaries or in determining whether specific simulation conditions have been met.

The For Loop includes a flowchart executed repeatedly as defined by the control variables and test conditions.



The Foreach Loop and While Loop stages allow for the introduction of control structures within a flowchart. In each case, allowing for the introduction of a complete flowchart to be executed repeatedly until the foreach vector (like `{T,P}`) of variables is exhausted, or the while condition is no longer true.

The Foreach Structure Loop takes structures contained in a Structures List or a previous Trajectory and performs on each of these structures the same calculation protocol as defined in the Foreach Structure Loop flowchart.

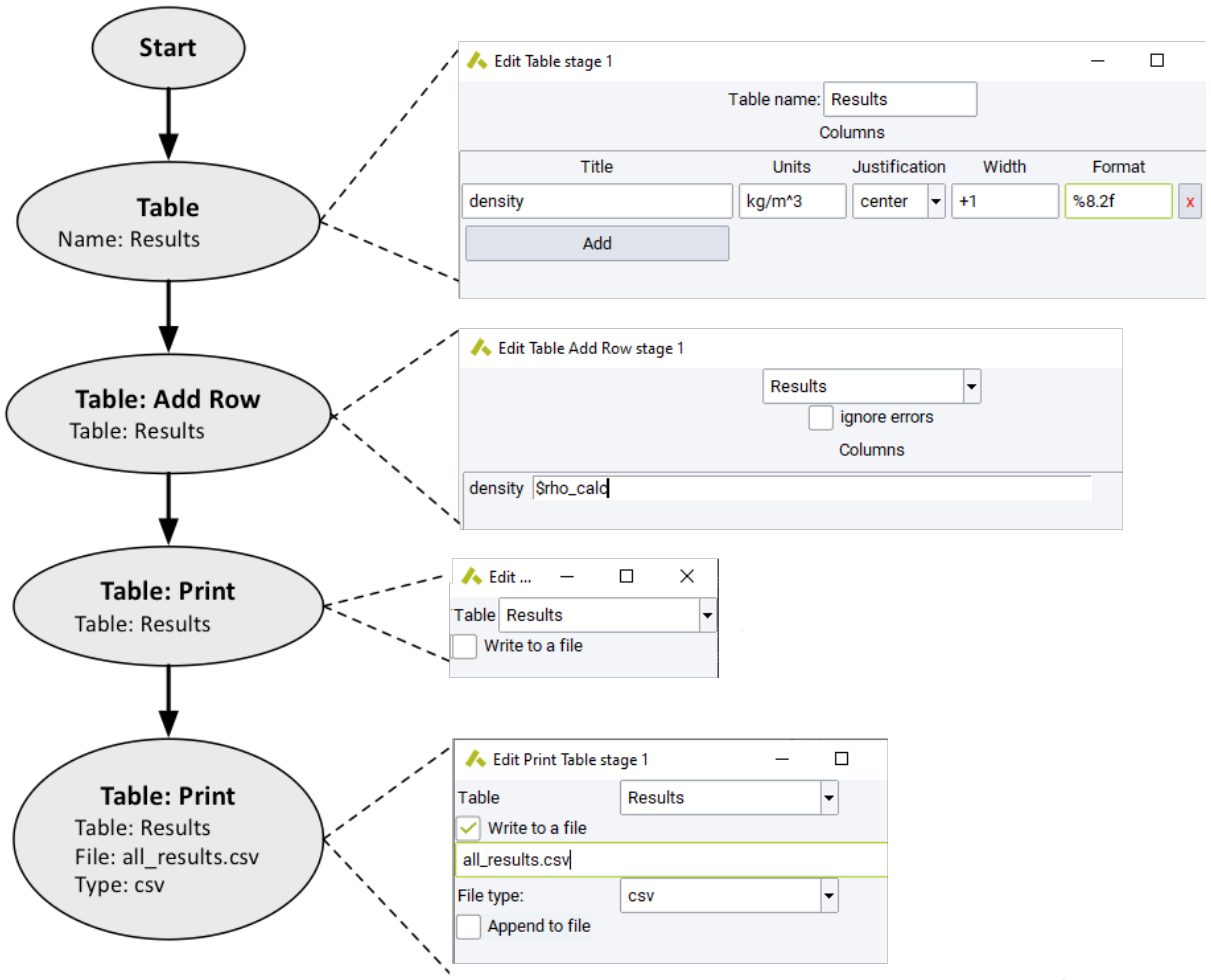
The loops are either synchronous, meaning that each iteration is completed before the next is started, or asynchronous, where multiple iterations run in parallel. Asynchronous operation mode is switched on by checking Run the different loop iterations simultaneously, specifying the degree of parallel operation by the parameter Maximum number of jobs to submit simultaneously. All looping structures have an option to Catch and ignore errors in the iterations.

The Catch stage allows for more elaborate error handling, that is in case the flowchart runs into an error, it is caught and another flowchart executed.

The If stage allows execution of a flowchart, if a condition is true (then), or an alternative flowchart (else).

3 Tables and Graphs

This section allows do define a Table, insert results as soon as they occur with Add Row and finally Print the entire table. The flowchart below is just an illustration, leaving out all looping and calculation.



With Table you define a Table by giving it a name and adding columns. Each column has a

- `Title`: Name of the column
- `Units`: Results are converted into units chosen. If no unit is specified, the default unit is used.
- `Justification`: Left, right, or center
- `Width`: How much "space" on the left and right
- `Format`: Can be provided in the printf format. For example; `%d` or `%i` for integer values, `%f` for float/double values, `%c` for characters, `%s` for strings, and `%x` for hexadecimal values.

Hint: The maximum number of characters/digits that can be used to print a given variable can be defined by an integer value between the `%` sign and the character. In case of a float value two numbers, separated by a comma, can be used. In this case the second number defines the number of digits after the comma used to print the value. For example, `%8.2f` displays a floating point variable with up to 8 characters in total and two digits after the comma.

Table: Add Row adds a line of results to a specified table. Variables can be added, in accordance with the Tcl paradigm, by adding a `$` sign in front of the variables name, e.g., the variable `Etotal_calc` can be printed with `$Etotal_calc` into a table.

Table: Print the selected Table. You can also save or append the result to a file as formatted text, comma separated values (csv), tab-delimited , or delimited by a different Separator like `;`.

4 General Properties

Mechanical Properties determines the mechanical properties with LAMMPS or VASP based on given Strains. For more information refer to the chapter on the Theory of elasticity.

Hill-Wallpole bounds: applies Hill-Walpole statistics on top of Mechanical Properties (see the section on Hill-Walpole bounds for amorphous systems).

Effective Mass: uses VASP to determine the effective mass for a specified k-point. For a more detailed description of the use of this stage see the section on Accurate Effective Mass calculations.

5 Methods

The Methods section of the flowchart interface provides access to a computational engine such as GIBBS, LAMMPS, MOPAC, GAUSSIAN or VASP (VASP flowcharts or a stage accessing the VASP GUI otherwise accessible from the Tools menu). In each case, the interface provided allows you to start a new flowchart, and execute relevant specific commands within this new flowchart.

In addition, there are methods available making use of the computational engines above to calculate vibrational properties (Phonon), to optimize cluster expansions for alloy and other disordered systems and perform Monte Carlo simulations for larger ensembles (UNCLE), to predict properties of polymers using correlations (P3C) or group contributions (QSPR), and to optimize force field parameters by fitting to ab-initio data (FFO).

Additional information on each of the Methods available in this section of the flowchart interface is available in the section of the User's Guide dealing with each method.

6 Building and Editing

Flowchart building commands allow for the construction and adjustment of atomic models.

6.1 Set Cell

The Set Cell stage permits the adjustment of unit cell dimensions for periodic systems. Here a variety of options are supported, the density or volume may be specified, or an expansion factor applied to the current system, or specific unit cell dimensions set. This stage may be combined with an appropriate Foreach Loop to explore the volumetric or density specific behavior of a given system property.

6.2 Change periodicity

A stage to turn on or remove periodic boundary conditions. In this stage the specify a gap to leave between the periodic building blocks. This stage may be used to combine a non periodic calculation, for example with MOPAC, with a periodic VASP calculation.

6.3 Supercell

The Supercell command may be applied to increase the size of a given model. As this building process is executed on the JobServer this is an efficient mechanism to create large systems.

6.4 Amorphous builder

The Amorphous Builder stage can be used to create amorphous models. *System composition source* can be set to the current system, where the current structure is split into molecules and recombined, to composition files saved on the local machine, and to a composition used in a previous job with jobserver. The *system geometry* of the amorphous material can be either bulk cell or layer and is build according to the set Temperature and cell dimensions. The later is set with *specify cell* and can be a mixture of the specific cell dimensions a, b, and c in combination with density. Accordingly additional options become available. The number of mols of the defined composition is set with *Nmols*. As this is a stochastic process the *number of configurations* that are to be created can be set. Multiple amorphous structures can be used to determine the average property of a given model. See the chapter on Amorphous Materials Builder for more information.

6.5 Thermoset Builder

The Thermoset Builder creates a densely crosslinked thermoset structure from an equilibrated bulk amorphous system. The crosslinking process involves the creation of bonds between user specified sets of atoms (*sites*), achieved in a series of crosslinking cycles through the growth of a *capture sphere* about each site.

During each cycle, bonds are created between reacting pairs of atoms lying within each site's capture sphere until the maximum allowed number of connections specified for each site has been reached. After cleaning to remove high energy interactions, each cycle is completed by performing structural relaxation using a small number of iterations of molecular dynamics followed by minimization.

The process continues through the growth of the capture sphere until either a maximum realistic radius has been reached, or until other specified conditions prevail (exceeding a maximum number of cycles, the maximum extent of reaction, threshold strain energy in the system, or detection of catenations between small rings).

Note that the Thermoset Builder operates on a principle analogous to that of the Polymer Builder. Thus, whereas the Polymer Builder operates by connecting together polymer repeat units rather than monomers (e.g. -(CH $_2$-CH $_2$)- rather than H $_2$C=CH $_2$for polyethylene), the Thermoset Builder creates crosslinks in a pre-cured system of network fragments (e.g. H $_2$N-R-NH $_2$and H $_3$C-CH(OH)- CH $_2$-O-R'-O-CH $_2$-CH(OH)-CH $_3$for an epoxy resin system, where the terminal nitrogens of the amine are sites capable of making up to two connections and the terminal carbons of the diglycidyl ether fragment are sites each capable of reacting once).

Note: The extent of reaction of a given site type is the total number of crosslinks formed at/by sites of that type (e.g. type 'A'), divided by the total number of crosslinks possible at those sites, with the latter being equal to the product of the total number of sites of a given type and the maximum number of bonds that can be created at the site defined by, for example, Site A max reactions.

Whenever the Maximum extent of reaction criterion is exceeded at the end of a crosslinking cycle, the builder will stop. Moreover, if the crosslinked system is stoichiometrically unbalanced, the criterion applies to sites of the component present in excess.

6.6 Parameters

Required input parameters are as follows:

Number of crosslink site types: A value of 1 would be used to mimic self-crosslinking (e.g. as produced by irradiation), while more commonly a value of 2 would be used to simulate reactions such as those involved in epoxy resin curing.

Site A subset: *MedeA* subset name for a set of crosslinkable sites.

Site A max reactions : number of new bonds between sites of type A and other sites. Note that after adding each new bond, a hydrogen atom is removed from the site A atom.

Site A substitution effect prob : Whenever the site can participate in more than a single crosslinking reaction, this list of parameters can be used to control the relative probability of successive reactions at the site. For example, a site capable of participating in two reactions (such as an amine first transformed from primary to secondary, and then from secondary to tertiary) may utilize this parameter to specify the relative probability of crosslink formation at sites which have reacted once already relative to those which have never reacted. By extension, relative reaction probabilities at a site capable of participating in N reactions would be specified by giving a list of (N-1) probabilities, which will often take the form of a list of decreasing values. Note that for common amine-cured epoxy thermosets, the relative rates of secondary and primary amine reactions may often lie in the range 0.2-0.6 for aromatic amines, with larger values for aliphatic amines (see, for example, *"Cross-linking of Epoxy Resins", K. Dusek, in Rubber-modified thermoset resins ACS Adv. Chem. Ser. vol 208 (1984)*).

Site B subset : second subset when two site types have been specified.

Site B max reactions : maximum number of connections to a type B site.

Site B substitution effect prob : See explanation of the analogous parameter for sites of type A.

Allowed reactions : between the two types of sites, only displayed when more than one site type is used. Most commonly this will only be between the different types of site.

Beginning capture radius ; in Angstroms applied at the start of the crosslinking process.

Capture radius increment : capture sphere radius is increased when no bondable pairs are found to lie within the current sphere for all sites.

Relaxation conditions : Indicates whether the relaxation dynamics applied at the end of each cycle are to be performed under constant volume (NVT) or constant pressure (NPT) conditions.

Relaxation iterations (per cycle): sets the total amount of structural relaxations.

Note: The use of a large value ($>$10) will significantly increase the time taken to perform the crosslinking, and is best used for very rigid systems.

Maximum extent of reaction : is the fraction of the maximum possible reactions reached, at which the building will stop.

Maximum capture radius : capture radius at which the building will stop.

Maximum crosslinking cycles : reduce the number of cycles below that implicitly defined by the maximum, beginning and capture radius increment.

Stop at gelation : Selecting this option will cause the building to terminate immediately after the formation of a 3-dimensional infinite network has been detected, overriding other termination parameters such as the Maximum extent of reaction . This can be useful for studying the gel point itself, and for examining the properties of the network immediately after formation.

Reset Forcefield atom types : this checkbox is selected by default and indicates that forcefield atom types and partial charges will be reassigned following completion of the building, which will often be necessary prior to performing further LAMMPS simulations due to changes in the bonded environment of individual atoms resulting from crosslink formation. Uncheck the option if you wish to exercise complete control over atom types and partial charges.

Write structure after each cycle : If this checkbox is selected, the coordinates and topology of the relaxed structure at the end of each crosslink cycle will be saved in a *MedeA* trajectory file for later visualization or further manipulation.

Control intramolecular ring formation : Enabling this option can be useful for studying how intramolecular reactions influence network structure and properties such as the gel point or behavior such as elastic constants and thermal conductivity of the final network.

Minimum ring size (atoms) : This parameter is only required when limiting intramolecular ring formation is to be applied. Typically, rings containing a small number of atoms are most likely to be formed (where allowable sizes are determined by the bonding topology of the reactants). Consequently, specifying a value equal to 'n+1', where 'n' denotes the number of atoms in the smallest ring, will exclude only those rings form the network. Conversely, specifying a large value will practically eliminate all intramolecular cycles.

Properties

This stage generates building related information, including maximum bond strain, and dimensionality of the structure as a function of progress of the crosslinking (see `Progress.txt` and `bondEnergy.png` on the Job's page). A dimensionality of 3 denotes that the gel point has been exceeded and that a true 3-Dimensional network has been created.

Note: Restarting crosslinking from a partially crosslinked system is not yet supported.

6.7 Translate Atoms

The Translate Atoms command can be used to adjust the position of atoms within the current system. Thereby it is possible to explicitly select atoms of the active structure or to select a subset. Atoms can be translated by a translation vector or to a point. The displacement can be in fractional or cartesian coordinates.

6.8 Docking

The Docking stage combines two structures. The host structure is the 'stream' structure upon which the Flowchart is operating. The Guest from Job is specified as the final.sci of the specified job on the current Job Server, the Host is specified as the input structure submitted with the flowchart. Number of guests defines how many guest molecules are put into the host, for each guest this process is repeated for Maximum iterations. The Maximum displacement (Ang) should be larger than the diameter of any ring to avoid interlocking of molecules. Scale rotations by and Temperature (K) as well as the underlying theory is explained in the section on Docking.

6.9 Randomly Substitute Atoms

Replaces a defined number of atoms, accounting for the symmetry of the structure, of *element A* with either *vacancies* or atoms of *element B*. For more information refer to the section on Random Substitution.

6.10 Simple Dynamics & Minimization

This stage uses the same simple dynamics and minimization algorithm that is also accessible from the MedeA GUI. The Number of dynamics steps and the Number of minimization steps can be set separately. Use this stage to pre-optimize a structure before applying a computationally more demanding algorithm to it.

6.11 Subset Manager

Manipulate existing subsets in a structure.

7 Structures Lists

These are a collection of commands to handle Structures Lists:

New List creates a new structure list that is accessible by the current flowchart. The List name and the File name of the structure lists can be defined. If no subfolder is specified the list will be placed in the job folder. The list can be initialized from an initial list that is saved locally on the machine running the MedeA GUI. Note, that multiple structure list can be active at the same time.

Save to List adds the current structure to any of the active structure lists. In addition, the structure can be saved with multiple properties.

Extract from List will extract a structure, specified by Structure index and Configuration index, from any of the active lists.

Sort List will sort any of the active structure lists according to a specific property.

Remove Duplicates from List remove all duplicates from a given list. Duplicates are identified by making use of symmetry.

Compute Descriptors on a list define and compute descriptors on a list.

Apply QSAR model on List by loading the equation from a XML QSAR model file.

8 Forcefield

Set Forcefield allows you to specify a forcefield.

Assign Atom Types and Charges allows you to readjust or set atomic forcefield parameters. This requires a forcefield with auto-typing.

Note: When using a custom forcefield in conjunction with a remote JobServer it is required that the forcefield is placed in the identical directory on the JobServer. To facilitate this, it is recommended to place the custom forcefield in a directory named `Forcefields/custom` located in Linux under {`/home/username`}`/MD/2.0/data`. On Windows save it to `C:/MD/2.0/data/Forcefields/custom`.

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9 Analysis

Orientation determines the orientation of a subset to a given reference vector:(x , y ,:highlightgray:*z*).

10 Properties

Below listed properties are made available in the flowchart after a specified stage. To access any of these use a `$` sign in front of the property name. For example, the variable `Etotal_calc` can be accessed with `$Etotal_calc`.

10.1 *MedeA* LAMMPS

DOCUMENTATION

Table1: All calculation types (last structure)

Property	Units	averaged
t_calc	fs	no
T_calc	K	yes
P_calc	atm	yes
V_calc	$Å^3$	yes
rho_calc	g/mL	yes
Etotal_calc	kcal/mol	yes
Epot_calc	kcal/mol	yes
Ekin_calc	kcal/mol	yes
Evdw_calc	kcal/mol	yes
Ecoul_calc	kcal/mol	yes
Enonbond_calc	kcal/mol	yes
Ebond_calc	kcal/mol	yes
EAngle_calc	kcal/mol	yes
Edihed_calc	kcal/mol	yes
Eimp_cal	kcal/mol	yes
Eint_calc	kcal/mol	yes
a_calc	Å	yes
b_calc	Å	yes
c_calc	Å	yes
alpha_calc	0	yes
beta_calc	0	yes
gamma_calc	0	yes
Sxx_calc	atm	
Syy_calc	atm	yes
Szz_calc	atm	yes
Syz_calc	atm	yes
Sxz_calc	atm	yes
Sxy_calc	atm	yes
deltaQ_calc.	kcal/mol	no
dQ/dt_calc	kcal/mol/fs	yes
deltapx_calc	Å/fs*g/mol	no
dpx/dt_calc	Å/fs*g/mol/fs	yes
CED_calc	J/cm^3	yes
CEDvdw_calc	J/cm^3	yes
CEDcoul_cal	J/cm^3	yes
dHvap (ideal)_calc	kJ/mol	yes
nSteps_calc		no
Fmax_calc	kcal/mol/Å	no
Frms_calc	kcal/mol/Å	no
P_calc	atm	no
V_calc	$Å^3$	no
rho_calc	g/mL	no
Sxx_calc	atm	no
Syy_calc	atm	no
Szz_calc	atm	no
Syz_calc	atm	no
Sxz_calc	atm	no
Sxy_calc	atm	no

10.2 *MedeA* VASP

Different properties are calculated depending on the type of VASP calculation configured within the VASP stage. Properties listed in the first table are always available after a successful VASP calculation.

Table2: All calculation types (last structure)

Property	Units	Description
Eelectronic_calc	eV	VASP energy (for primitive cell)
Eelectronic_calc	eV	VASP energy (for primitive cell)
Eelectronic_conventionalCell_calc	eV	VASP energy (for conventional cell)
Eelectronic_empiricalFormula_calc	eV	VASP energy (for empirical formula)
Eelectronic_sigma0_calc	eV	VASP energy extrapolated to zero smearing (for primitive cell)
Enon-dispersive_calc	eV	VASP energy without van der Waals contribution, if van der Waals forcefield is applied *(for primitive cell)*
EVanderWaals_calc	eV	VASP energy, van der Waals contribution, if van der Waals forcefield is applied (for primitive cell)
FormulaPrimitiveCell_calc		Formula of the primitive cell
FormulaConventionalCell_calc		Formula of the conventional cell
FormulaEmpirical_calc		Empirical formula
FactorEmpiricalToPrimitive_calc		Factor to convert empirical formula to primitive cell formula
FactorEmpiricalToConventional_calc		Factor to convert empirical formula to conventional cell formula
Efermi_calc	eV	Fermi energy
a_calc	$\mathring{A}$	Lattice parameter a
b_calc	$\mathring{A}$	Lattice parameter b
c_calc	$\mathring{A}$	Lattice parameter c
alpha_calc	degree	Lattice parameter
beta_calc	degree	Lattice parameter
gamma_calc	degree	Lattice parameter
Vprim_calc	$\mathring{A}^3$	Volume (primitive cell)
rho_calc	Mg/m^3	Density
mu_calc	μ_B	Total magnetic moment (spin-polarized)
mux_calc	μ_B	Total magnetic moment in x direction (spin-orbit or non-collinear magnetic)
muy_calc	μ_B	Total magnetic moment in y direction (spin-orbit or non-collinear magnetic)
muz_calc	μ_B	Total magnetic moment in z-direction (spin-orbit or non-collinear magnetic)
Eformation_calc	kJ/mol	Formation energy
Hformation_calc	kJ/mol	Heat of formation
approximateMaterial_calc		Type of material: metal, semiconductor or insulator
approximateGap_calc	eV	Band gap width
approximateGapType_calc		Type of band gap: direct, indirect, no
approximateVBMaxPosition_calc		Approximate position of the valence band maximum in the Brillouin zone (fractional coordinates of a vector in k-space)
approximateCBMinPosition_calc		Approximate position of the conduction band minimum in the Brillouin zone (fractional coordinates of a vector in k-space)
return_status_calc		Return status: finished, warnings, error
planewaveCutoff_calc	eV	Plane wave cutoff
nKPoints_calc		Number of k-points in the Brillouin zone
FFTGridX_calc		Coarse Fast-Fourier grid in x direction
FFTGridY_calc		Coarse Fast-Fourier grid in y direction
FFTGridZ_calc		Coarse Fast-Fourier grid in z direction
FFTFineGridX_calc		Fine Fast-Fourier grid in x direction
FFTFineGridY_calc		Fine Fast-Fourier grid in y direction

Continued on next page

Table 2 – continued from previous page

Property	Units	Description
FFTFineGridZ_calc		Fine Fast-Fourier grid in z direction
FFTAddedGridX_calc		Extrafine Fast-Fourier grid in x direction added for evaluation of augmentation charges and accurate forces
FFTAddedGridY_calc		Extrafine Fast-Fourier grid in y direction added for evaluation of augmentation charges and accurate forces
FFTAddedGridZ_calc		Extrafine Fast-Fourier grid in z direction added for evaluation of augmentation charges and accurate forces
FFTCompleteGridX_calc		Minimum Fast-Fourier grid in x direction to avoid aliasing errors
FFTCompleteGridY_calc		Minimum Fast-Fourier grid in y direction to avoid aliasing errors
FFTCompleteGridZ_calc		Minimum Fast-Fourier grid in z direction to avoid aliasing errors

Table3: Single Point and Structure Optimization (optimized structure)

Property	Units	Description
V_calc	$\mathrm{\AA}^3$	Volume (conventional cell)
P_calc	GPa	Pressure
Sxx_calc	GPa	Stress tensor component xx
Syy_calc	GPa	Stress tensor component yy
Szz_calc	GPa	Stress tensor component zz
Syz_calc	GPa	Stress tensor component yz
Sxz_calc	GPa	Stress tensor component xz
Sxy_calc	GPa	Stress tensor component xy

DOCUMENTATION

Table4: Ab initio Molecular Dynamics

Property	Units	Description
Etotal_calc	kJ/mol	Total energy (average)
Etotal_uncertainty_calc	kJ/mol	Total energy (standard deviation)
Ekin_calc	kJ/mol	Kinetic energy (average)
Ekin_uncertainty_cal	kJ/mol	Kinetic energy (standard deviation)
Epot_calc	kJ/mol	Potential energy (average)
Epot_uncertainty_calc	kJ/mol	Potential energy (standard deviation)
V_calc	$Å^3$	Volume (average)
V_uncertainty_calc	$Å^3$	Volume (standard deviation)
P_calc	GPa	Pressure (average)
P_uncertainty_calc	GPa	Pressure (standard deviation)
T_calc	K	Temperature (average)
T_uncertainty_cal	K	Temperature (standard deviation)
Sxx_calc	GPa	Stress tensor component xx (average)
Sxx_uncertainty_calc	GPa	Stress tensor component xx (standard deviation)
Syy_calc	GPa	Stress tensor component yy (average)
Syy_uncertainty_calc	GPa	Stress tensor component yy (standard deviation)
Szz_calc	GPa	Stress tensor component zz (average)
Szz_uncertainty_calc	GPa	Stress tensor component zz (standard deviation)
Syz_calc	GPa	Stress tensor component yz (average)
Syz_uncertainty_calc	GPa	Stress tensor component yz (standard deviation)
Sxz_calc	GPa	Stress tensor component xz (average)
Sxz_uncertainty_calc	GPa	Stress tensor component xz (standard deviation)
Sxy_calc	GPa	Stress tensor component xy (average)
Sxy_uncertainty_calc	GPa	Stress tensor component xy (standard deviation)

Table5: (Total, valence) charge density, Bader analysis

Property	Units	Description
BaderCharges_calc		electron charge. Bader charge per atom for each site
BaderChargeTransfers_calc		electron charge. Charge transfer per atom for each site
BaderVolumes_calc	$Å^3$	Bader volume per atom for each site
BaderDistances_calc	Å	Bader distance for each site
BaderVacuumCharge_calc		electron charge. Bader charge of the vacuum region
BaderVacuumVolume_calc	$Å^3$	Bader volume of the vacuum region
BaderTotalVolume_calc	$Å^3$	Total Bader volume

Table6: Density of states and Optical spectra

Property	Units	Description
DOS_approximateMaterial_calc		Type of material: metal, semiconductor or insulator
DOS_approximateGap_calc	eV	Band gap width
DOS_approximateGapType_calc		Type of band gap: direct, indirect, no
DOS_approximateVBMaxPosition_calc		Approximate position of the valence band maximum in the Brillouin zone (fractional coordinates of a vector in k-space)
DOS_approximateCBMinPosition_calc		Approximate position of the conduction band minimum in the Brillouin zone (fractional coordinates of a vector in k-space)
DOS_Efermi_calc	eV	Fermi energy
DOS_nKPoints_calc		Number of k-points in the Brillouin zone

Table7: Zone center phonons

Property	Units	Description
PhononFrequencyGamma_calc	THz	Phonon frequencies at the Γ-point from finite differences

Table8: Response tensors

Property	Units	Description
eps_0xx_calc		Dielectric constant e_0, xx component
eps_0yy_cal		Dielectric constant e_0, yy component
eps_0zz_calc		Dielectric constant e_0, zz component
eps_0yz_calc		Dielectric constant e_0, yz component
eps_0xz_calc		Dielectric constant e_0, xz component
eps_0xy_calc		Dielectric constant e_0, xy component
eps_infxx_calc		Dielectric constant $e_{infinity}$, xx component
eps_infyy_calc		Dielectric constant $e_{infinity}$, yy component
eps_infzz_calc		Dielectric constant $e_{infinity}$, zz component
eps_infyz_calc		Dielectric constant $e_{infinity}$, yz component
eps_infxz_calc		Dielectric constant $e_{infinity}$, xz component
eps_infxy_calc		Dielectric constant $e_{infinity}$, xy component
BornEffectiveCharges_calc		electron charge. 3x3 Born effective charges matrices for each atom position
PhononFrequencyGammaResponse_calc	THz	Phonon frequencies at the Γ-point from linear response
piezo_clampedion11_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 11
piezo_clampedion12_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 12
piezo_clampedion13_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 13
piezo_clampedion14_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 14
piezo_clampedion15_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 15
piezo_clampedion16_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 16
piezo_clampedion21_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 21
piezo_clampedion22_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 22
piezo_clampedion23_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 23
piezo_clampedion24_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 24
piezo_clampedion25_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 25
piezo_clampedion26_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 26
piezo_clampedion31_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 31
piezo_clampedion32_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 32
piezo_clampedion33_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 33
piezo_clampedion34_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 34
piezo_clampedion35_cal	C/m^2	Piezoelectric tensor (clamped ion) comp. 35
piezo_clampedion36_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 36
piezo_relaxedion11_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 11
piezo_relaxedion12_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 12
piezo_relaxedion13_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 13
piezo_relaxedion14_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 14
piezo_relaxedion15_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 15
piezo_relaxedion16_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 16
piezo_relaxedion21_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 21
piezo_relaxedion22_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 22
piezo_relaxedion23_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 23
piezo_relaxedion24_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 24
piezo_relaxedion25_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 25
piezo_relaxedion26_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 26

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Property	Units	Description
piezo_relaxedion31_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 31
piezo_relaxedion32_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 32
piezo_relaxedion33_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 33
piezo_relaxedion34_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 34
piezo_relaxedion35_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 35
piezo_relaxedion36_calc	C/m^2	Piezoelectric tensor (clamped ion) comp. 36

Table9: Electric field gradients

Property	Units	Description
EFGs_Vxx_calc	V/Å^2	Electric field gradient for each atom, component xx
EFGs_Vyy_calc	V/Å^2	Electric field gradient for each atom, component yy
EFGs_Vzz_calc	V/Å^2	Electric field gradient for each atom, component zz
EFGs_Vyz_calc	V/Å^2	Electric field gradient for each atom, component yz
EFGs_Vxz_calc	V/Å^2	Electric field gradient for each atom, component xz
EFGs_Vxy_calc	V/Å^2	Electric field gradient for each atom, component xy
EFGs_diagonalized_Vxx_calc	V/Å^2	Electric field gradient diagonalized for each atom, component xx
EFGs_diagonalized_Vyy_calc	V/Å^2	Electric field gradient diagonalized for each atom, component yy
EFGs_diagonalized_Vzz_calc	V/Å^2	Electric field gradient diagonalized for each atom, component zz
EFGs_asymmetry_calc		Electric field gradient asymmetry parameter
NMRQuadrupolarParameters_calc		Nuclear quadrupolar parameter of each atom
NucElecQuadrupoleMoments_calc		Nuclear electric quadrupole moment of each atom

Table10: Hyperfine parameters

Property	Units	Description
HyperfineTotal_Axx_calc	MHz	Total hyperfine coupling parameter diagonalized for each atom, component xx
HyperfineTotal_Ayy_calc	MHz	Total hyperfine coupling parameter diagonalized for each atom, component yy
HyperfineTotal_Azz_calc	MHz	Total hyperfine coupling parameter diagonalized for each atom, component zz
HyperfineFermiContact_calc	MHz	Fermi contact (isotropic) hyperfine coupling parameter for each atom
HyperfineDipolar_Axx_calc	MHz	Dipolar hyperfine coupling parameters for each atom, component xx
HyperfineDipolar_Ayy_cal	MHz	Dipolar hyperfine coupling parameters for each atom, component yy
HyperfineDipolar_Azz_calc	MHz	Dipolar hyperfine coupling parameters for each atom, component zz
HyperfineDipolar_Ayz_calc	MHz	Dipolar hyperfine coupling parameters for each atom, component yz
HyperfineDipolar_Axz_calc	MHz	Dipolar hyperfine coupling parameters for each atom, component xz
HyperfineDipolar_Axy_calc	MHz	Dipolar hyperfine coupling parameters for each atom, component xy
HyperfineAsymmetry_calc	MHz	Hyperfine coupling asymmetry parameter

Table11: Work function (surfaces only)

Property	Units	Description
WorkFunction_calc	eV	Work function for identical terminations
WorkFunction_left_calc	eV	Work function for different terminations
WorkFunction_right_calc	eV	Work function for different terminations

Table12: Work function (surfaces only) - additional properties resulting from dipole correction

Property	Units	Description
DipoleMoment_calc	e Å	Dipole moment of the slab (vector)
TraceQuadrupoleMoment_calc		Trace of the quadrupole moment tensor
EcorrDipoleQuadrupole_calc	eV	Dipol+quadrupol energy correction
EcorrCharge_calc	eV	Energy correction for charged systems

10.3 *MedeA* Mechanical Properties / MT - Elastic Constants.

This applies to the Mechanical Properties stage and the MT - Elastic constants type of calculation in the VASP 5.4 stage

Property	Units	Description
Cij_calc(Cij)	GPa	Elastic constants C_{ij} (1 leqslant i,j leqslant 6)
Cij_uncertainty_calc(Cij)	GPa	Standard deviation for elastic constants C_{ij}
CijMatrix_calc	GPa	Elastic constants matrix (full 6x6 matrix)
SijMatrix_calc	1/GPa	Compliance tensor (full 6x6 matrix)
LeastSquaresResidual_calc		Residual % to which the least squares converged
ResidualStrain_calc(lat)		Residual strain (lat = a,b,c,alpha,beta,gamma)
PredictedCellParameter_calc(lat)	Å	Cell parameters predicted from the least squares fit (lat = a,b,c,alpha,beta,gamma)
MechanicalStabilityEigenValues_calc		Eigenvalues of the elastic constant matrix
MechanicalStabilityEigenVectors_calc		Eigenvectors of the elastic constant matrix
IsMechanicallyStable_calc		Whether mechanically stable (1) or not (0)
VoigtBulkModulus_calc	GPa	Bulk modulus from Voigt's average
ReussBulkModulus_calc	GPa	Bulk modulus from Reuss' average
HillBulkModulus_calc	GPa	Bulk modulus from Hill's average
VoigtShearModulus_calc	GPa	Shear modulus from Voigt's average
ReussShearModulus_calc	GPa	Shear modulus from Reuss' average
HillShearModulus_calc	GPa	Shear modulus from Hill's average
VoigtYoungsModulus_calc	GPa	Young's modulus from Voigt's average
ReussYoungsModulus_calc	GPa	Young's modulus from Reuss' average
HillYoungsModulus_calc	GPa	Young's modulus from Hill's average
VoigtLongitudinalModulus_calc	GPa	Longitudinal modulus from Voigt's average
ReussLongitudinalModulus_calc	GPa	Longitudinal modulus from Reuss' average
HillLongitudinalModulus_calc	GPa	Longitudinal modulus from Hill's average
VoigtPoissonRatio_calc	GPa	Poisson's ratio from Voigt's average
ReussPoissonRatio_calc	GPa	Poisson's ratio from Reuss' average
HillPoissonRatio_calc	GPa	Poisson's ratio from Hill's average
VoigtPughsRatio_calc	GPa	Pugh's ratio from Voigt's average
ReussPughsRatio_calc	GPa	Pugh's ratio from Reuss' average
HillPughsRatio_calc	GPa	Pugh's ratio from Hill's average
VoigtChenVickersHardness_calc	GPa	Vickers hardness according to Chen's model from Voigt's average

Continued on next page

Table 13 – continued from previous page

Property	Units	Description
ReussChenVickersHardness_calc	GPa	Vickers hardness according to Chen's model from Reuss' average
HillChenVickersHardness_calc	GPa	Vickers hardness according to Chen's model from Hill's average
VoigtTianVickersHardness_calc	GPa	Vickers hardness according to Tian's model from Voigt's average
ReussTianVickersHardness_calc	GPa	Vickers hardness according to Tian's model from Reuss' average
HillTianVickersHardness_calc	GPa	Vickers hardness according to Tian's model from Hill's average
TransverseSpeedOfSound_calc	m/s	Speed of sound of transverse waves
LongitudinalSpeedOfSound_calc	m/s	Speed of sound of longitudinal waves
SpeedOfSound_calc	m/s	Mean speed of sound
HaveSpeedOfSound_calc		Whether or not speed of sound is available (1/0)
DebyeTemperature_calc	K	Debye temperature (Hill's average)
MeltingTemperatureLindemann_calc	K	Melting temperature estimated from Lindemann's expression (Hill's average)
GrueneisenParameter_calc		Grüneisen parameter (Hill's average)
E0_calc	kJ/mol	Energy at 0K = electronic energy + zero-point energy
Epv_calc	kJ/mol	Energy contribution of the PV term
Ezp_calc	kJ/mol	Zero-point energy
H0_calc	kJ/mol	Enthalpy at 0 K = E0_calc + Epv_calc
Thermodynamic_calc(T)	K	Temperature grid for thermodynamic functions
Thermodynamic_calc(Cv)	J/K/mol	Constant volume heat capacity
Thermodynamic_calc(dH)	kJ/mol	Enthalpy, temperature dependent part
Thermodynamic_calc(dG)	kJ/mol	Gibbs free energy, temperature dependent part
Thermodynamic_calc(E)	kJ/mol	Internal energy including E0_calc
Thermodynamic_calc(H)	kJ/mol	Enthalpy including H0_calc
Thermodynamic_calc(G)	kJ/mol	Gibbs free energy
Thermodynamic_calc(A)	kJ/mol	Helmholtz free energy
Thermodynamic_calc(S)	J/K/mol	Entropy
Thermodynamic_calc(alpha)		Coefficient of thermal expansion

10.4 *MedeA* Phonon (Flowchart)

This applies to the Phonon stage, but not to the Phonon GUI (from the Tools menu), which cannot be integrated into a Flowchart

Property	Units	Description
E0_calc	kJ/mol	Energy at 0K = electronic energy + zero-point energy
Epv_calc	kJ/mol	Energy contribution of the PV term
Ezp_calc	kJ/mol	Zero-point energy
H0_calc	kJ/mol	Enthalpy at 0 K = E0_calc + Epv_calc
Thermodynamic_calc(T)	K	Temperature grid for thermodynamic functions
Thermodynamic_calc(Cv)	J/K/mol	Constant volume heat capacity
Thermodynamic_calc(dH)	kJ/mol	Enthalpy, temperature dependent part
Thermodynamic_calc(dG)	kJ/mol	Gibbs free energy, temperature dependent part
Thermodynamic_calc(E)	kJ/mol	Internal energy including *E0_calc*
Thermodynamic_calc(H)	kJ/mol	Enthalpy including *H0_calc*
Thermodynamic_calc(G)	kJ/mol	Gibbs free energy
Thermodynamic_calc(A)	kJ/mol	Helmholtz free energy
Thermodynamic_calc(S)	J/K/mol	Entropy

10.5 *MedeA* GIBBS

Table14: All calculation types

Property	Units	Description
Pvirial_calc_<phase>_<run>	MPa	Virial Pressure (NVT, NPT & only fluid in GCMC)
alphaT_calc_<phase>_<run>	1/Pa	Isothermal Compressibility (NPT)
cp_calc_<species>_<phase>_<run>	kJ/mol	Chemical Potential

Table15: NVT & NPT with test insertions, GEMC, GCMC

Property	Units	Description
Utot_calc_<species>_<phase>_<run>	kJ/mol	Average total potential energy (per mol of system)
ThermE_calc_<phase>_<run>	1/K	Thermal Expansivity (NPT)
Cpres_calc_<phase>_<run>	J/mol/K	Residual Heat Capacity (NPT constant Pressure)
U_el_calc_<phase>_<run>	kJ/mol	Average Electrostatic Energy (per mol of system)
N_calc_<phase>_<run>		Average total number of molecules
MVol_calc_<phase>_<run>	L/mol	Average molar volume
rho_calc_<phase>_<run>	Mg/m^3	Average phase density
vol_calc_<phase>_<run>	$Å^3$	Average phase volume
fug_calc_<species>_<phase>_<run>	Pa	Fugacity (NVT & NPT with test insertions, GEMC, GCMC)
U_el_grid_calc_<phase>_<run>	Pa	Average grid electrostatic energy (GCMC)
CompF_calc_<phase>_<run>		Isentropic compressibility coefficient Cp/Cv (NPT)
U_ext_calc_<phase>_<run>	kJ/mol	Average external energy (intermolecular energy)
DHvap_calc_<run>	kJ/mol	Vaporization Enthalpy

Table16: GEMC constant V, pure compounds

Property	Units	Description
x_calc_<species>_<phase>_<run>		Molar Fraction
JT_calc_<phase>_<run>	K/MPa	Joule-Thomson coefficient (NPT, Value for ideal heat capacity defined in flowchart)
vs_calc_<phase>_<run>	m/s	Speed of Sound (NPT, Value for ideal heat capacity defined in flowchart)

10.6 *MedeA* Gaussian

Property	Units	Description
Pvirial_calc_<phase>_<run>	MPa	Virial Pressure (NVT, NPT & only fluid in GCMC)
alphaT_calc_<phase>_<run>	1/Pa	Isothermal Compressibility (NPT)

Table17: Single point energy and geometry optimization

Property	Units	Description
Energy_total_calc	Ha	The total energy of the system
charge_calc	e	The total charge of the system
spin_multiplicity_calc		The spin multiplicity of the system
basis_calc		The basis set used
calculation_type_calc		Gaussian's representation of the calculation type
method_calc		Gaussian's representation of the calculation method
route_calc		The route section of the input file
mulliken_charges_calc(%ATOMID%)	e	The Mulliken charge of atom %ATOMID%

If the calculation uses a post-Hartree-Fock method then an appropriate subset of the following total energies and corrections will also be available, where a correction indicates the contribution to the total energy from the specified level of theory only. All energies have units of Hartree.

energy_scf_calc energy_mp2_calc energy_mp3_calc energy_mp4dq_calc energy_mp4sdq_calc energy_mp4sdtq_calc energy_ccsd_calc energy_ccsdt_calc energy_ccsdt_e4t_calc energy_mp2_correction_calc energy_mp3_correction_calc energy_mp4dq_correction_calc energy_mp4sdq_correction_calc energy_mp4sdtq_correction_calc energy_ccsd_correction_calc energy_ccsdt_correction_calc energy_ccsdt_e4t_correction_calc

If the calculation uses either Hartree-Fock or density functional theory then the dipole and quadrupole moments are also available. The dipole moment has units of e*a0 and the quadrupole moment has units of e*a0^2.

dipole_moment_au_calc(x) dipole_moment_au_calc(y) dipole_moment_au_calc(z)
dipole_moment_magnitude_calc quadrupole_moment_au_calc(xx)
quadrupole_moment_au_calc(xy) quadrupole_moment_au_calc(xz)
quadrupole_moment_au_calc(yy) quadrupole_moment_au_calc(yz)
quadrupole_moment_au_calc(zz)

Table18: Frequencies (available after a frequencies calculation)

Property	Units	Description
mode_numbers_calc		A list of the included mode numbers
mode_symmetries_calc		A list of the included mode symmetries
mode_frequencies_calc	1/cm	A list of mode frequencies
mode_IR_intensities_calc	km/mol	A list of IR intensities
mode_reduced_masses_calc	u	A list of the reduced masses
force_constants_calc	mDyne/Ang	A list of the force constants
low_frequency_modes_calc	1/cm	The lowest frequencies in the system, corresponding to translations and rotations
enthalpy_thermal_correction_calc	Ha	The thermal correction to the enthalpy
gibbs_free_energy_thermal_correction_calc	Ha	The thermal correction to the Gibbs free energy
zero_point_energy_calc	Ha	The zero point energy
inertia_principle_axes_calc		A list of the principle axes of inertia
inertia_principle_moments_calc	me/a0^2	A list of the principle moments of inertia
rotational_constants_calc	GHz	The rotational constants
rotational_temperatures_calc	K	The rotational temperatures
pressure_calc	atm	The calculation pressure
temperature_calc	K	The calculation temperature
apt_charges_calc(%ATOMID%)	e	The APT charge of atom %ATOMID%

If the calculation method has analytic derivatives, which may not be the case for higher order Moller-Plesset or coupled cluster calculations, a frequencies calculation also produces a dipole and quadrupole moment. The dipole moment has units of e*a0 and the quadrupole moment has units of e*a0^2.

dipole_moment_au_calc(x) dipole_moment_au_calc(y) dipole_moment_au_calc(x)
dipole_moment_magnitude_calc quadrupole_moment_au_calc(xx)
quadrupole_moment_au_calc(xy) quadrupole_moment_au_calc(xz)
quadrupole_moment_au_calc(yy) quadrupole_moment_au_calc(yz)
quadrupole_moment_au_calc(zz)

If the calculation method has analytic second derivatives (and hence analytic frequencies - HF, DFT and MP2), which includes the HF, DFT and MP2 methods, a frequencies calculation also yields the polarizability and hyperpolarizability (both in atomic units) and APT charges.

polarizability_au_calc(xx) polarizability_au_calc(xy) polarizability_au_calc(xz) polarizability_au_calc(yy) polarizability_au_calc(yz) polarizability_au_calc(zz) hyperpolarizability_au_calc(xxx) hyperpolarizability_au_calc(xxy) hyperpolarizability_au_calc(xxz) hyperpolarizability_au_calc(xzz) hyperpolarizability_au_calc(xyy) hyperpolarizability_au_calc(xyz) hyperpolarizability_au_calc(yyy) hyperpolarizability_au_calc(yyz) hyperpolarizability_au_calc(yzz) hyperpolarizability_au_calc(zzz)

Polarizability

Variables available after a frequencies calculation include all of those from a commensurate single point energy calculation and the dipole moment and polarizability. The dipole moment has units of e*a0 and the polarizability is in atomic units.

dipole_moment_au_calc(x) dipole_moment_au_calc(y) dipole_moment_au_calc(x) dipole_moment_magnitude_calc polarizability_au_calc(xx) polarizability_au_calc(xy) polarizability_au_calc(xz) polarizability_au_calc(yy) polarizability_au_calc(yz) polarizability_au_calc(zz)

If the calculation method is either Hartree-Fock or density functional theory then a polarizability calculation also produces the hyperpolarizability in atomic units.

hyperpolarizability_au_calc(xxx) hyperpolarizability_au_calc(xxy) hyperpolarizability_au_calc(xxz) hyperpolarizability_au_calc(xzz) hyperpolarizability_au_calc(xyy) hyperpolarizability_au_calc(xyz) hyperpolarizability_au_calc(yyy) hyperpolarizability_au_calc(yyz) hyperpolarizability_au_calc(yzz) hyperpolarizability_au_calc(zzz)

10.7 Additional Notes on Flowcharts

- The final structure obtained in the previous stage is passed to each subsequent stage. Hence, the end point of an NPT calculation, for example, is passed to the next stage in a simulation.
- The principal computed results are placed in local variables accessible by subsequent stages. The names of these variables are formed from the name of the property, with `_calc`, `_uncertainty_calc` and `_converged_calc` appended in the case of averages.
- The input and output files associated with each stage in a particular Job are stored on the JobServer. The directory hierarchy employed beneath each individual Job reflects the structure of the flowchart, which was employed in that calculation.