Transport Modules

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1 Functionality for the component:

Transport modules are used to compute flux-surface-averaged heat fluxes, particle fluxes and, in some cases, momentum transport fluxes across magnetic surfaces. The neoclassical transport module is also used to compute the neoclassical electrical resistivity and bootstrap current density, which are used in the magnetic diffusion equation. In addition, some of the anomalous transport modules are also used to compute anomalous contributions to equipartition (such as the local energy flow between electrons and ions, for example).

The flux-surface-average transport equations can be written for the charged particle density of each species n_s

$$\frac{1}{V'}\frac{\partial(V' n_s)}{\partial t}\bigg|_{\psi_{\rm tor}} + \langle \nabla \cdot \mathbf{\Gamma_s} \rangle = S_s, \tag{1}$$

for the toroidal momentum density of each species $m_s n_s \langle R v_{s\,\rm tor} \rangle$

$$\frac{1}{V'}\frac{\partial(V' m_s n_s \langle R v_{s\,\rm tor} \rangle)}{\partial t}\bigg|_{\psi_{\rm tor}} + \langle \nabla \cdot \mathbf{\Pi_s} \rangle = R_s, \tag{2}$$

for the energy density of each species $3 n_s T_s / 2$

$$\frac{3}{2}\frac{1}{(V')^{5/3}}\frac{\partial[(V')^{5/3} n_s T_s]}{\partial t}\bigg|_{\psi_{\rm tor}} + \langle \nabla \cdot \mathbf{q_s} \rangle = Q_s, \tag{3}$$

In these transport equations, V is the volume within a flux surface labelled by ρ and $V' \equiv \partial V / \partial \rho$. The partial derivatives with respect to time are taken relative to flux surfaces with constant toroidal flux $\psi_{\rm tor}$. The particle flux, $\mathbf{\Gamma_s}$, momentum flux, Π_s, and heat flux, $\mathbf{q_s}$ are all defined relative to surfaces of constant toroidal flux, as are the particle source rate, S_s, momentum source rate, R_s, and energy source rate, Q_s, for each species s. (These transport equations, then, automatically predict the correct adiabatic compression effects when flux surfaces move rapidly on the transport time scale.) The flux surface average operator $< \ldots >$ will be defined in the next subsection.

The magnetic diffusion equation for the poloidal magnetic flux $\psi_{\rm pol}$

$$\left.\frac{\partial \psi_{\rm pol}}{\partial t}\right|_{\psi_{\rm tor}} = \frac{\eta R B_{\rm tor}}{\mu_o V' \langle 1/R^2 \rangle} \frac{\partial}{\partial \rho} \left[\frac{V'}{R B_{\rm tor}} \left\langle \frac{|\nabla \rho|^2}{R^2} \right\rangle \frac{\partial \psi_{\rm pol}}{\partial \rho} \right] + S_\psi. \tag{4}$$

is normaly solved separately because it usually evolves on a much slower time scale. In this equation, η is the electrical resistivity, μ_o is the vacuum magnetic permeability $[4\pi \times 10^{-7}$ volt $\cdot$ sec / (amp $\cdot$ meter)], R is the major radius, $B_{\rm tor}$ is the toroidal magnetic field (note that $RB_{\rm tor}$ is uniform over flux surfaces), and S_ψ is the non-inductive source of poloidal flux (from current drive, for example).

Consider a flux surface label, ρ, that increases monotonically from the magnetic axis to the edge of the plasma. Usually, ρ is taken to be

$$\rho \equiv \sqrt{\psi_{\rm Tor}/\psi_{\rm Tor\ edge}}, \tag{5}$$

where $\psi_{\rm Tor}$ is the toroidal flux through any cross section of a magnetic surface, and $\psi_{\rm Tor\ edge}$ is the corresponding toroidal flux at the edge of the plasma (or at the separatrix). Using this definition, it follows that ρ increases monotonically from 0.0 at the magnetic axis to 1.0 at the edge of the plasma

It can be shown that the expression for the flux surface average of the thermal fluxes can be written

$$\langle \nabla \cdot \mathbf{q_s} \rangle = \frac{\partial}{\partial V} \langle \nabla V \cdot \mathbf{q_s} \rangle = \frac{1}{V'} \frac{\partial (V' \langle \mathbf{q_s} \cdot \nabla \rho \rangle)}{\partial \rho}. \tag{6}$$

There are corresponding equations for the divergence of the particle fluxes $\langle \nabla \cdot \mathbf{\Gamma_s} \rangle$ and the divergence of the momentum fluxes $\langle \nabla \cdot \mathbf{\Pi_s} \rangle$.

In most applications, the transport fluxes are separated into a diffusive part, with thermal diffusivity χ_s, and a convective part, with thermal convective velocity $\mathbf{v}_s$, where the subscript s denotes the species. If the heat flux is written in the form

$$\mathbf{q}_s = -\chi_s n_s \nabla T_s - n_s T_s \mathbf{v}_s, \tag{7}$$

then the flux surface average of the divergence of the heat flux becomes

$$\langle \nabla \cdot \mathbf{q}_s \rangle = -\frac{1}{V'} \frac{\partial}{\partial \rho} \left[V'(\rho) \left(\left\langle |\nabla \rho|^2 \right\rangle \chi_s n_s \frac{\partial T_s}{\partial \rho} + \langle |\nabla \rho| \rangle \, n_s T_s \mathbf{v}_s \right) \right]. \tag{8}$$

Hence, the metric elements $\langle|\nabla\rho|^2\rangle$ and $\langle|\nabla\rho|\rangle$ appear explicitly in the transport equations.

In the case of neoclassical transport [1] and classical transport, where all of the fluxes are linear functions of the density, momentum and temperature gradients, it is a straightforward matter to separate the fluxes into diffusive and convective parts. In the case of most anomalous transport models, however, where the fluxes are very non-linear functions of the gradients, there is no unique way to separate the fluxes into diffusive and convective parts. It is found that the performance of the transport equation solver can be strongly affected by the way that this separation is carried out, even though the resulting fluxes are independent of the way they are split into diffusive and convective parts. The transport driven by ion temperature gradient (ITG) or electron temperature gradient (ETG) turbulence, for example, is found to be "stiff", which means that the transport fluxes increase rapidly with increasing ion temperature gradient (in the case of the ITG mode) or increasing electron temperature gradient (in the case of the ETG mode), once these gradients exceed a critical threshold which depends upon other plasma parameters such as the density gradient, magnetic shear and plasma beta.

In quasi-liner models, such at the GLF23 model [2] or the MMM95 Multi-Mode model [3], the core algorithms compute the fluxes of heat, particles and, in some cases, momentum. (As a matter of convenience, the output variables for some of the transport modules are "effective" diffusivities, which are just the fluxes divided by the corresponding gradients. It is a simple matter to convert from effective diffusivities back to the more fundamental fluxes.) The separation between diffusive and convective parts is normally carried out by using a finite difference approximation to take the derivative of each flux with respect the gradients of the temperatures (and sometimes the gradients of the densities). However, some of the diffusivities (particularly particle diffusivities) that are computed by this algorithm can be negative under some conditions. Since negative diffusivities result in ill posed transport equations, the diffusive part of the flux is normally all converted to a convective part of the flux under these conditions.

2 Determine the minimum interface to provide this functionality.

Most of the transport models that have been developed to date are local in the sense that all of the input is, in principle, local to each flux surface. However, the Mixed-Bohm/gyro-Bohm transport model [4] is inherently non-local, in the sense that the electron and ion thermal transport throughout the plasma depends on a finite difference approximation to the electron temperature gradient across 20% of the plasma radius near the plasma edge. It is expected that other transport models in the future will be inherently non-local since gyro-kinetic turbulence simulations indicate that the turbulence is coupled across the plasma. The list of input variables given below applies to most of the existing transport models and then exceptions are noted for those models that do not fit the normal patern. In most cases, the modules accept a radial array for each profile.

2.1 Plasma species

In some transport modules, such as NCLASS [1] and a new version of the extended drift wave model, each ionization state of each plasma species is treated separately and is characterized by an atomic number, nuclear charge, charge state, and isotope mass (usually expressed in AMU). However, in most of the transport modules in the National Transport Code Collaboration (NTCC) Module Library [5], an effective hydrogenic (or main) ion species and an effective impurity ion species are each characterized by a density-weighted average charge state and atomic mass. There is normally a separation between the thermal species (electrons, main ions and impurity ions) and the fast (super-thermal) species, such as neutral beam inected ions or fast alpha particles.

Normally, densities are prescribed for each thermal ion species and a fast ion species. The electron density is computed assuming quasi-neutrality

$$n_e = \sum_i Z_i n_i \tag{9}$$

where Z_i and n_i are the charge state and density of each ion species, including thermal and fast ions. This quasi-neutrality condition also imposes a local constraint on the normalized gradients of the densities. Since the charge states are normally positive and the ion densities are always positive, the electron density computed by Eq. 9 is always positive. Some transport codes follow the evolution of the electron density and then compute one of the ion densites from the quasi-neutrality condition. In that case, it is important to choose one of the dominant ion densities to be computed from the quasi-neutrality condition, so that the computation does not involve a small difference between small numbers or the possibly of a negative density.

In addition to the density for each species, the temperature and, in some modules, the toroidal velicity or momentum for each species are inputs to the transport modules. Normally, density weighted averages are used when an effective species consists of several sub-species that are lumped together. The average fast ion energy density is used for fast ion species.

Normalized gradients, such as

$$g_{T_i} \equiv -R(\partial T_i/\partial r)/T_i \tag{10}$$

where R is the major radius and r is the flux surface half-width, are required inputs for most of the transport modules. There are several reasons for requiring the gradients in addition to the underlying plasma variables or profiles. First, it is useful to be able to evaluate the transport computed by modules one flux surface at a time in order to compare transport modules in stand-alone codes. Second, some transport codes smooth the normalized gradients in order to control numerical instabilities that are commonly produced by stiff transport models. Third, different transport codes use different representations for the profiles from the magnetic axis to the edge of the plasma. For example, some transport codes allow for a non-uniform radial grid spacing and finite element techniques can be used rather than a simple finite difference technique. Hence, the authors of many of the transport modules allow the user to compute normalized gradients outside of the module and to pass the normalized gradients as input variables.

The normalized gradient is used rather than the gradient scale length,

$$L_{T_i} \equiv R/g_{T_i} = T_i/(\partial T_i/\partial r)$$

because the gradient scale length becomes infinite as the normalized gradient passes through zero. In any finite difference or finite element representation used in transport codes, the gradient of any plasma profile is never infinite.

2.2 Flow shear rate

Most anomalous transport modules allow the $E \times B$ flow shear rate

$$\omega_{E\times B} = \frac{(RB_{\rm pol})^2}{B} \frac{\partial}{\partial \psi} \left(\frac{E_r}{RB_{\rm pol}} \right) \tag{11}$$

to be computed externally and passed as an input variable. The GLF23 module has an option to compute the flow shear rate internally given the toroidal angular velocity and the parallel and the component of the perpendicular velocity within the flux surface.

2.3 Metric elements and magnetics

Usually, the fundamental flux surface label used in most transport codes is ρ defined by Eq. 5, where $\rho = 0.0$ at the magnetic axis and $\rho = 1.0$ at the edge of the plasma. There are two interleaved grids used in most 1-1/2-D integrated modeling codes. The transport fluxes and the magnetics profiles, such as the magnetic q profile, are computed on the zone boundaries grid. Temperatures, densities and other thermodynamic plasma profiles are computed on zone centers, which are spaced half way between zone boundaries. In effect, the plasma is divided up into cells, which are called zones, and the zone boundaries define the edges of the zones while the zone centers characterize the interior of the zones.

In addition to the flux surface label ρ, many of the transport modules also require each flux surface half-width, major radius, elongation, and, in some cases, triangularity. In some transport modules, it is specified that the major radius corresponds to the geometric center of the flux surface, while in other transport modules, the major radius is computed at the outboard edge of the flux surface, where most of the transport is generated by turbulence that has a strongly ballooning character. It is normally expected that the toroidal magnetic field is given at the same point that the major radius is computed.

Some of the transport modules require the metric elements $\langle|\nabla\rho|\rangle$ and $\langle|\nabla\rho|^2\rangle$, which are needed to split the fluxes into diffusive and convective parts, as described above. The neoclassical module, NCLASS [1], requires $\langle|B|^2\rangle$, $\langle 1.0/|B|^2\rangle$, $\langle|\nabla\rho|^2/B^2\rangle$, and $\langle\hat{n}\cdot\nabla\theta\rangle$, where B is the magnetic field strength at each point around the flux surface, $\hat{n}$ is a unit vector normal to the flux surface, and θ is a poloidal angle-like variable with $0 \le \theta \le \pi$

around the flux surface. The NCLASS and MMM95 modules also require the trapped particle fraction on each flux surface.

Most of the transport modules expect the magnetic q value on each flux surface as input. Normally, the magnetic q value is taken to mean the true Shafranov q-value, which is the ratio of toroidal magnetic winding number to poloidal winding number. Many transport modules also require the magnetic shear as input. Different modules use different definitions of magnetic shear.

2.4 Non-local variables

As pointed out above, the Mixed-Bohm/gyro-Bohm transport model [4] requires a finite difference approximation to the electron temperature gradient across 20% of the plasma radius near the plasma edge. In addition, the neoclassical transport module NCLASS [1] requires some variables evaluated at the magnetic axis such as $\kappa(0) B_{\rm toroidal}(0)/(2q(0)^2)$ and $q(0)R(0)$, where $\kappa(0)$ is the elongation of the magnetic surface at the magnetic axis. The GLF23 module requires the toroidal flux at the last closed flux surface.

Most transport modules accept nearly all of the input variables as arrays representing the profiles across the plasma.

2.5 Control switches

The options in most of the transport modules can be controlled by setting arrays of integer and real-valued control switches. Usually, the options that are available to non-expert users are limited, while options available to expert users allow for detailed diagnostics and model development.

2.6 Output variables

Essentially all of the transport modules compute flux-surface-averaged electron and ion thermal heat fluxes. In addition, most of the modules compute particle fluxes. Some of the modules also compute the momentum fluxes (such as GLF23 and a recent version of the Weiland model) or the electrical resistivity and the bootstrap current density (in the case of NCLASS). In many of the transport modules, the transport fluxes are subdivided for diagnostic purposes into the component fluxes produced by each mode of turbulence (such as transport driven by the ITG or ETG or resistive ballooning mode). In most transport codes, the fluxes are split into diffusive and convective parts, as described in Section 1 above.

3 Identify code specific data

Examples of specific switch settings and usage are illustrated in the driver program that is included with each NTCC module. In addition, researchers in the field have acquired experience with the implementation of the transport modules within their own integrated modeling codes.

4 What expectations or assumptions that the component will have about the data it gets from another component

As described above, the transport modules generally expect profile arrays of plasma variables as a function of flux surface from the magnetic axis to the edge of the plasma. Many of the transport modules are written as a set of nested routines, in which the inner routines use normalized input variables to compute normalized transport fluxes on a single flux surface. Outer routines then convert the fluxes to diffusivities (in m^2/sec) and convective velocities (in m/sec) over the array of flux surfaces.

Some of the transport models are very sensitive to some of the input variables. For example, the stiff models based on ITG turbulence are sensitive to the normalized gradient of the ion temperature.

5 Identify possible shared infrastructure ...

The quasi-linear modules use the same generalized eigenvalue and eigenfunction solver.

6 Identify physics analysis/development needs and identify possible mathematical or algorithmic problems or opportunities for improvement. Identify additional opportunities for parallelism that are not presently realized.

The main issue concerns the development of a solver for advancing the transport equations when using very stiff tranpsort models. Experience has indicated that the way in which the fluxes are split into diffusive and convective parts has a large effect on the efficiency and accuracy of the solver. There can be severe problems when the transport modules produce negative diffusivities, which happens, in particular, for the particle diffusivities.

When the transport modules are strictly local, or when they depend on non-local information in a simple way, they can be parallelized by computing the transport on each flux surface on a different processor.

7 Summary of computational needs this component will have when used for the fast MHD campaign — including computations, memory, amount of time to carry out its designated task in the framework, and kind of parallelism (threaded or distributed memory or both).

References

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