Status on the computational aspects of developing a fully gyrokinetic transport code

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PROJECT OVERVIEW

> The goal of this project is to develop a prototypical steady state gyrokinetic transport (SSGKT) code that integrates micro-scale gyrokinetic turbulence simulations into a framework for practical multi-scale simulation of the International Thermonuclear Experimental Reactor (ITER).

The prototype will have the capability to predict steady-state core temperature and density profiles given the H-mode pedestal boundary conditions. This addresses a key problem of critical scientific importance; namely predicting the performance of ITER given an edge boundary condition.

The key numerical challenge is to determine the most efficient feedback algorithm, because code outputs are intermittent and extremely expensive.

The key scientific advance will be to show that gyrokinetic codes (simulating micro-scales) can be run practically within a transport code (simulating the macro-scale). This is referred to as simulation of turbulence on transport timescales and is cited as one of the four leading Focused Integration Initiatives for a Fusion Simulation Project[3].

OLD APPROACH

Presently, at the *macro-scale* end of the spectrum, predictive modeling of steady-state temperature and density profiles [4] is usually done with simplified local transport models like GLF23 [5], which are based on rather approximate fits to the results of linear and nonlinear simulations.

At the *micro-scale* end the spectrum, the standard approach in the gyrokinetic simulation community is to compute the statistical steady-state of turbulence [2] which is generated by *fixed* plasma profiles.

GYRO is regularly used for fixed-profile simulations (i.e., without feedback) of global DIII-D, JET, C-MOD and NSTX experiments. Such simulations are far shorter than the global transport (energy confinement) time.

NEW APPROACH

By separating the turbulence (internal, micro-scale physics) and transport (external, macro-scale physics) time scales, and introducing a feedback loop between them, one can arrive at the steady-state transport balance required for a true macro-scale steady-state solution. We will use a master coupler code to coordinate and provide feedback between a transport code and multiple separate GYRO [1] simulations.

Each instance of GYRO will compute local radial fluxes that will be periodically communicated to the master. In comparison to the size of a local simulation distribution function, the amount of data to be communicated to the master will be minimal.

The coupler code and transport code are in development. The particular feedback scheme (or schemes) they will employ have not yet been decided.

The physical sources (beam ions, radio frequency heating, radiation, thermonuclear rates, etc.) which must be accounted for in the master are available as off-the-shelf technology.

The use of the transport power and plasma flow balance equation, rather than direct dynamical interactions, is potentially the key solution to connecting core turbulence to the edge pedestal.

> This new approach will allow highly efficient use of several thousand processors; the master code must only compute relatively simple feedback information based on transport power balance, and the independent instances of GYRO will scale very well because of the relatively low processor count per instance (32 to 256).

GYRO OVERVIEW

GYRO is a 5-D gyrokinetic-Maxwell solver which computes the radial transport of particles and energy $(\Gamma_\sigma and \chi_\sigma)$ using an implicit-explicit Runge-Kutta scheme discretized on an Eulerian grid

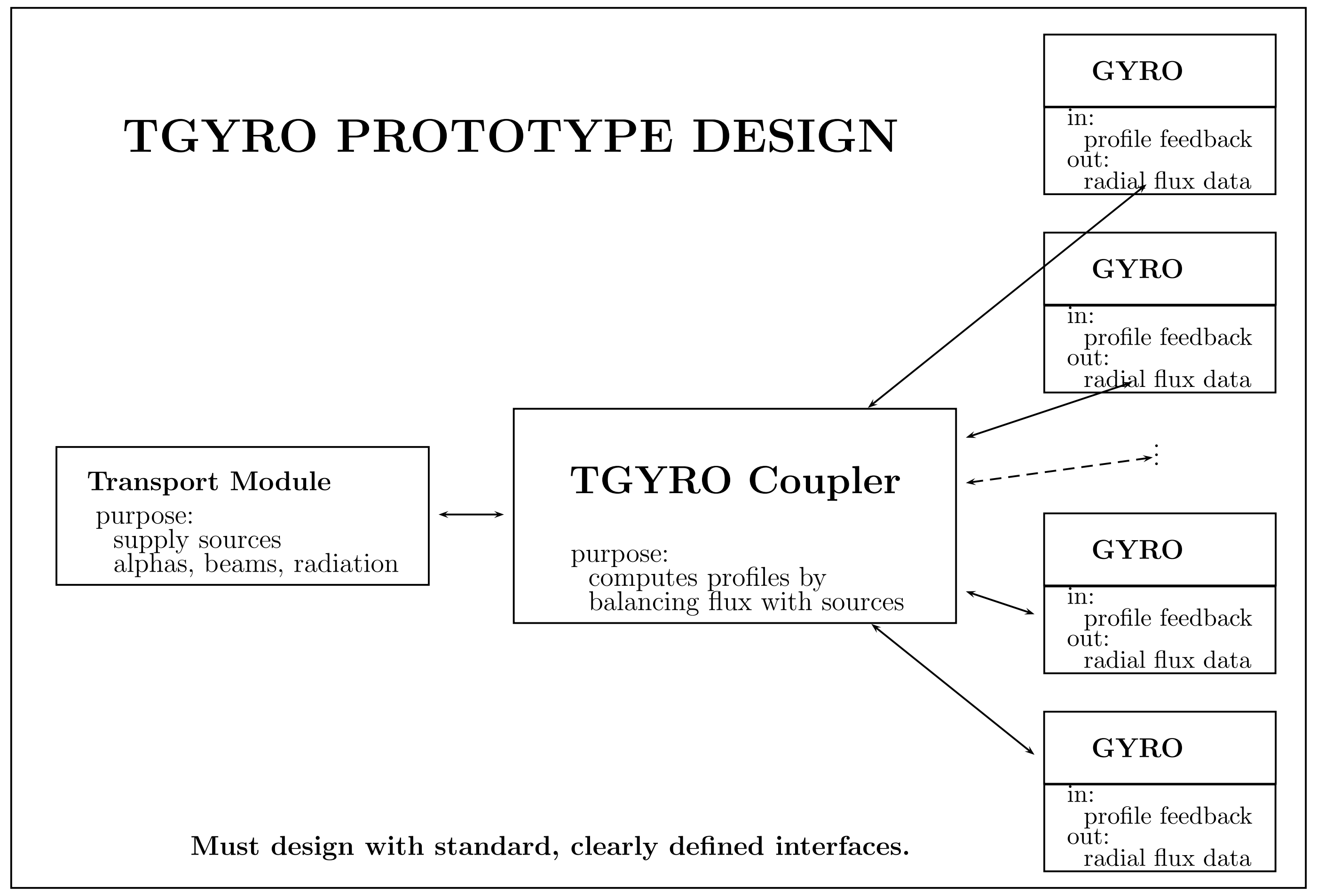
$$\frac{\partial f}{\partial t} = L_a f + L_b \Phi + \{f, \Phi\} \qquad \text{where} \qquad F\Phi = \iint dv_1 dv_2 \, f.$$

COMPUTER SCIENCE CHALLENGES

The project is funded by SciDAC through the Office of Advanced Scientific Computing Research. We are working with the Framework Application for Core-Edge Transport Simulations (FACETS) of which we are a Scientific Application Partnership (SAP).

We intend that the software framework we form will lay a foundation for even more powerful and comprehensive simulations in the future. We will strive to develop prototypical standards (interfaces) for fusion application modules, which will allow incorporation of other modern fusion applications codes into the framework.

Furthermore, we will need to resolve: (1) exactly what data needs to be communicated between the two codes, and (2) what is the most efficient way to communicate such data. Data exchanged among the models may reside on differing spatial meshes, requiring interpolation between the source and target components respective grids. The models may also differ in how they discretize time, requiring some scheme to either interpolate or average/accumulate data for translation between the source and target components' time meshes.



TGYRO PROTOTYPE DESIGN

Transport Module
purpose:
supply sources
alphas, beams, radiation

TGYRO Coupler
purpose:
computes profiles by
balancing flux with sources

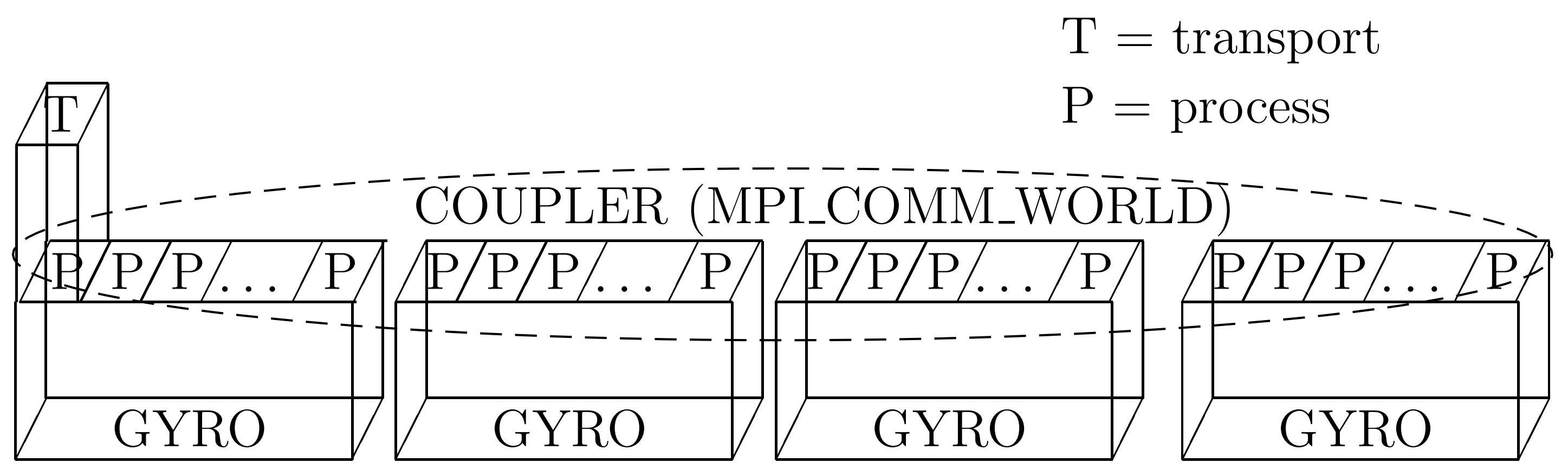
GYRO
in:
profile feedback
out:
radial flux data

Must design with standard, clearly defined interfaces.

PROTOTYPE MPI TASK MODEL

Our TGYRO prototype will have the following characteristics:

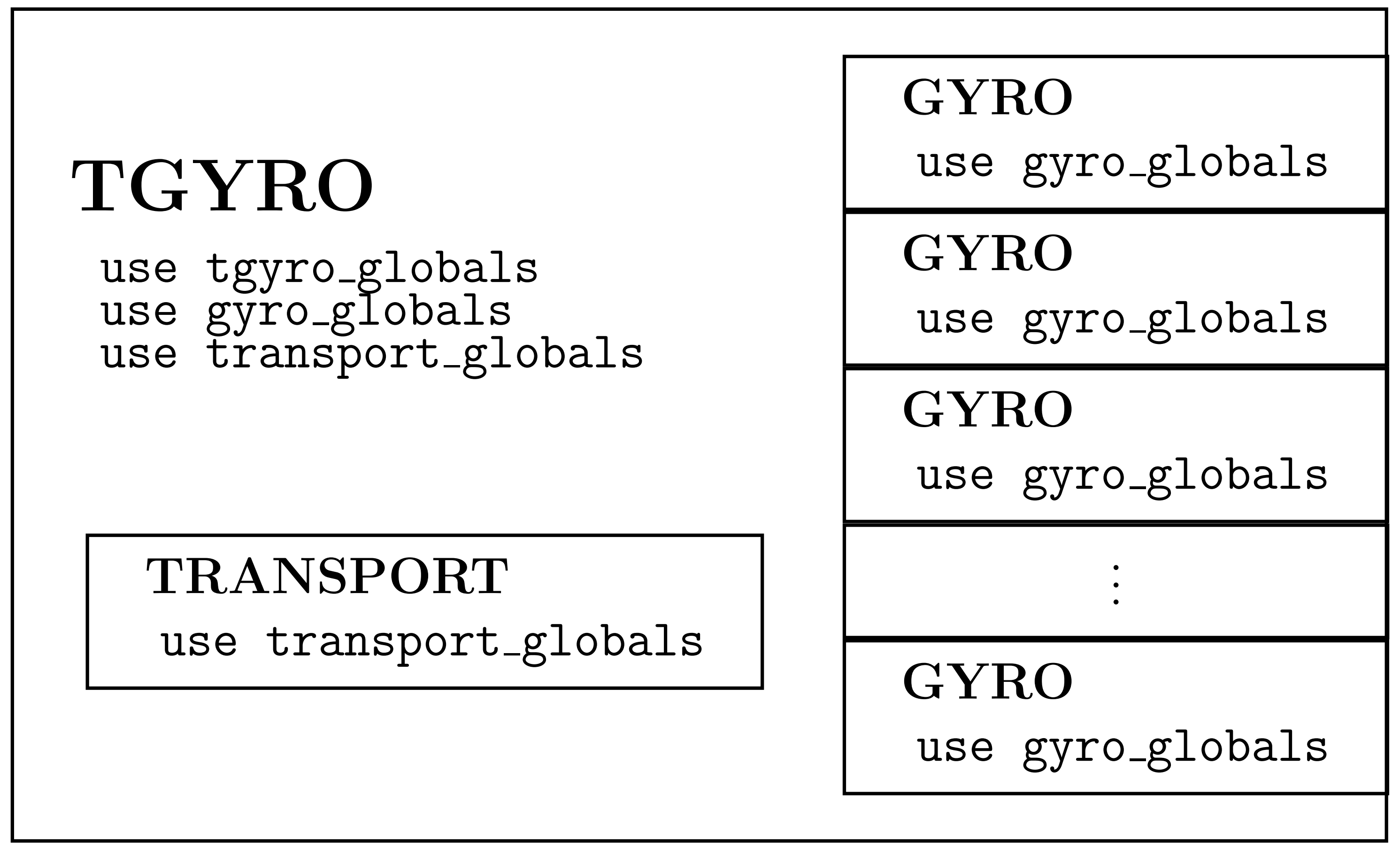
1. The coupler will initialize all MPI tasks from MPI_COMM_WORLD.
2. Create subcommunicators, say GYRO_COMM_WORLD for each GYRO instance. We envision that all the GYRO instances will be running concurrently.
3. After some predetermined number of timesteps, the GYRO instances will stop and return profile and gradient information that the coupler will massage, and reduce down to a master process.
4. This master process will then run the transport code and after determining the transport, return to the coupler and distribute.



T = transport
P = process

PROTOTYPE MEMORY MODEL

With our TGYRO prototype, we have decided to take advantage of modern Fortran modules for communicating data between the gyrokinetic and transport models. We are building a master coupler that will use three Fortran modules containing: 1) coupler variables, 2) GYRO variables, and 3) transport variables. Thus, the coupler will "know" the current state of every variable from both the gyrokinetic and transport models.



TGYRO

```
use tgyro_globals
use gyro_globals
use transport_globals
```

TRANSPORT

```
use transport_globals
```

GYRO

```
use gyro_globals
```

With this design, the "exchange of data" is quite simple and immediate. The coupler will need to interpolate and redistribute data as the gridding changes from gyrokinetic to transport and vice/versa, thus it will be very efficient since the coupler has all the data available at any given time.

SUMMARY

At this time, we have developed a TGYRO coupler code that can run multiple GYRO instances concurrently. The prototype is very portable and runs on all the platforms that GYRO already runs on. Furthermore, TGYRO employs a very similar build and execution mechanisms to the GYRO code, so existing GYRO users will find it easy to use.

A 4-radial node test has already been demonstrated. This test ran four multiple GYRO simulations within the TGYRO framework. The simulations were iterated (input parameters adjusted) to bring them into flux "balance" (production balances turbulent loss) with thermonuclear production. This was the first example of a steady-state profile prediction from a gyrokinetic code.

The next phase CS phase is to integrate a transport code into the TGYRO prototype. We expect that the transport code will be a modern Fortran code that uses modules and so the memory model explained above will be used. If not, we will "communicate" information via subroutine arguments after the transport code is subroutinized.

Numerical issues such as the design of a robust feedback scheme between the transport and gyrokinetic modules is an outstanding future challenge. These issues go hand-in-hand with defining interfaces for transport and gyrokinetic codes for which we hope to propose standards as the prototype matures.

References

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