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# Investigation of efficient and reliable numerical algorithms for coupled reactor calculations

X-TREAM project: Task 1a
Survey of the different numerical algorithms used in present computer codes.
Core simulators and core thermal-hydraulics.

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**Abstract**

Nowadays, the precise modeling of a nuclear reactor core is a challenge. This task involves several aspects, from the computational power needed to perform simulations, to the physics and analysis of the outcome. The need to better understand the physical phenomena is a critical issue in order to quantify and qualify nuclear safety parameters. Currently, substantial research has been done in order to optimize the prediction capabilities of coupled codes. The understanding of the multi-physics of coupled codes is also essential because of the strong coupling between the neutronics and the thermal-hydraulics. In this report a state of the art of current coupled codes is presented. The purpose of this is to present the main algorithms that independent and coupled codes use. By doing that, a better understanding of the numerical schemes is achieved, providing a consistent knowledge in order to select an appropriate algorithm to be implemented. This is the foundation of the X-TREAM project, which final objective is the improvement on the numerical algorithms used in coupled calculations.

Keywords: Core simulators, multi-physics, multi-scales, core thermal-hydraulics, coupled codes, numerical schemes.

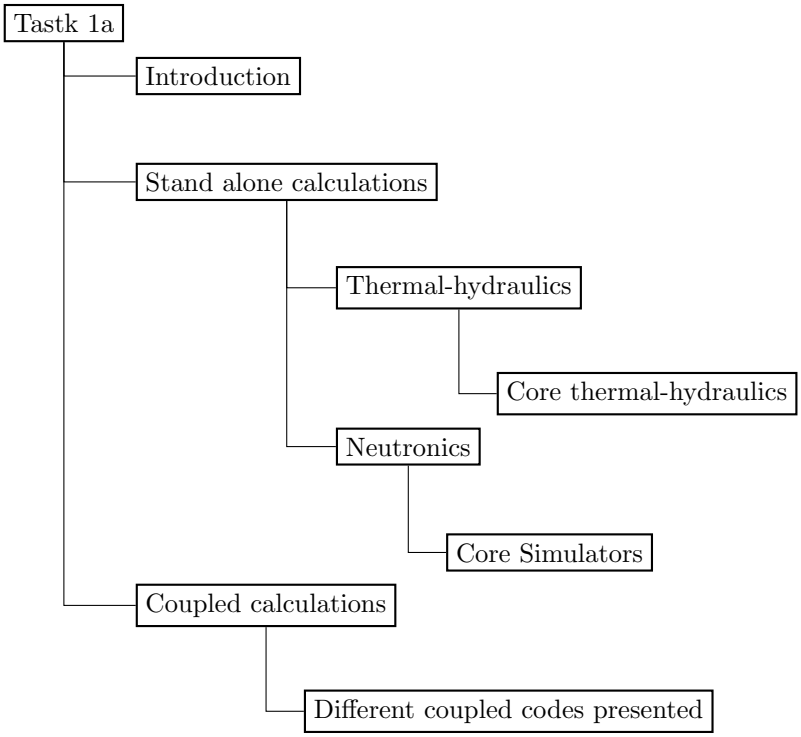


Figure 1: Structure of the report - Task 1b: Survey of the different numerical algorithms used in present computer codes.

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# 1 Acronyms

| | |
|---|---|
| ABN: | Approximated Block Newton |
| ACMFDM: | Analytic Coarse Mesh finite Difference Method |
| ADF: | Assembly Discontinuity Factors |
| ATWC: | Anticipated Transient Without all Control rods |
| ANM: | Analytical Nodal Method |
| ATWS: | Anticipated Transient Without SCRAM |
| BiCGSTAB: | Bi-conjugated gradient |
| BWR: | Boiling Water Reactor |
| CFD: | Computational Fluid Dynamics |
| CMFD: | Coarse Mesh Finite Difference |
| DNBR: | Departure from Nuclear Boiling Ratio |
| FD: | Finite Differences |
| FV: | Finite Volumes |
| FEM: | Finite Elements Method |
| FDS: | Finite Difference Schemes |
| FDM: | Finite Differences Method |
| FEBE: | Forward Euler Backward Euler |
| FPI: | Fixed Point Iteration |
| GE: | General Electric |
| GMRES: | Generalized Minimal RESidual |
| HEM: | Homogeneous Equilibrium Model |
| HPLWR: | High Performance Light Water Reactor |
| HRM: | Homogeneous Relaxation Model |
| ICE: | Implicit Continuous Eulerian |
| INL: | Idaho National Laboratory |
| JFNK: | Jacobian-Free-Newton-Krylov |
| LOCA: | Loss Of Coolant Accident |
| LWR: | Light Water Reactor |
| MED: | Memory Exchage Data |
| MOX: | Mixed OXide |
| MSL: | Main Steam Line |
| MSLB: | Main Steam Line Break |
| N: | Neutronics |
| NEM: | Nodal Expansion Method |
| NPP: | Nuclear Power Plant |
| OS: | Operator Splitting |
| OSSI: | Operator Split Semi Implicit |
| PBP: | Physics Base Preconditioner |
| PDE: | Partial Differential Equation |
| PVM: | Parallel Virtual Machine |
| PWR: | Pressurized Water Reactor |
| RPV: | Reactor Pressure Vessel |
| SCRAM: | Safety Control Rod Axe Man |
| SLB: | Steam Line Break |
| SOR: | Successive Over Relaxation |
| TH: | Thermal-Hydraulics |

# 2 Introduction

Accurate simulations for nuclear power plants (NPPs) have become more practical with the rapid growth of computing capabilities and with improved algorithms. Especially, coupling of codes is a beneficial approach for safety analysis. The understanding of the interaction between neutronics (N) and thermal-hydraulics (TH) is important in order to achieve the precise prediction of local parameters. In addition, numerical tools describing different physical phenomena have to be coupled between each other for analyzing e.g. normal plant conditions as well as loss of coolant accidents (LOCAs), reactivity transients, and anticipated transients without SCRAM (ATWS). Many of the current codes used for light water reactor (LWR) analysis are based on 3D nodal N methods coupled with first order 1D TH without considering cross flows [1]. The deterministic modeling performed today relies on the coupling of existing codes. The most mature multi-physical coupling scheme is the coupling of nodal diffusion codes with system codes and/or with 1D simplified TH codes using a rigid mapping scheme between codes. This coarse spatial discretization of both N and TH does not allow to describe local phenomena. In fact, due to the multi-scale and multi-physics features of LWRs, detailed modeling of nuclear reactors for the whole system and all scales is still not feasible. The necessity to better describe the most important physical phenomena prevailing in modern core loadings of LWRs with increasing heterogeneity is driving the extension of current core designs and N/TH coupled transient analysis methodologies. These improvements consider a more detailed spatial description of both N and TH computational domains and also the development of flexible coupling approaches as well as the use of improved diffusion or higher order approximations of the neutron transport equation.

Different groups in Europe and worldwide are working on the development of novel coupling approaches for multi-physics nuclear reactor simulations e.g. in the European Union the Nuclear Reactor Integrated Simulation Project (NURISP) [2] [3], included in the $6^{th}$ EURATOM framework program, in the USA, the MOOSE project [4], NNR [5] [6], CASL project [7], the Criticality Safety Package (CRISTAL) [8], and the Highly Evolutionary Methods for Extensive Reactor Analysis (HEMERA), developed by the Commissariat à l'Énergie Atomique (CEA) in collaboration with Institut National de Recherche et de Sécurité (INRS). In Sweden, research groups at KTH, Chalmers, and the industry (Westinghouse Electric Sweden AB), also lead the development of this kind of coupling approaches. The type of research that the Division of Nuclear Engineering at Chalmers is pursuing, is based on the multi-physics nature of nuclear reactors by taking it into account from the beginning of the modeling process. The Division of Nuclear Engineering at Chalmers has long been active in the deterministic modeling of nuclear reactors and a Deterministic REActor Modeling (DREAM) task force was created in 2013 in order to tackle the modeling of nuclear reactors from an innovative point of view. The DREAM task force deals with the investigation, improvement and development of numerical methods and techniques which take the multi-scale and multi-physics aspects of nuclear reactors. The benefits of these efforts directly impact the economics, both from an operational point of view as well as from a reactor analysis point of view. The operational advantages would be the possibility to run the nuclear reactors closer to their safety limits, as a result of a better evaluation of the safety margins. This in itself would lead to a more sustainable use of the nuclear fuel and the corresponding natural resources. The main goal of the project is the development of innovative computing and modeling techniques for advanced nuclear reactor safety evaluations. The project is targeted at investigating the existing different simulation strategies, which could later on be used in future simulation platforms. The sub-project that wraps and leads the current work is the X-TREAM project. This project, which stands for the "neXt generation numerical Techniques for deterministic REActor Modeling" is supported by the NORTHNET (Nordic Thermal-Hydraulic Network).

The purpose of this work is to give a clear idea of the characteristics of the main codes used nowadays worldwide. This task involves not only the understanding of stand alone codes, but also their coupling schemes (between N and TH). Is necessary to mention, that more details about these coupling schemes and other type of discretization are given in the report named, "Survey of the state of the art numerical techniques for solving coupled non-linear equations," devoted to the task 1b of the previously mentioned X-TREAM project. This report is divided in three main blocks. The first one involves the description of stand alone TH codes, the most popular used nowadays. The second block presents the most popular neutronic codes (focusing on core simulators), and the last section is devoted to the description of coupled codes and their general coupling schemes. The following figure illustrates the structure of the report.

# 3 Survey of the different numerical algorithms used in present computer codes

Nowadays one could find several computer codes that solve the time-dependent neutron diffusion and/or transport equation coupled with TH codes. Such N codes are for instance, DYN3D [9] , COBAYA3 [10], PARCS [11] and POLCA7 [12]. This coupling is done with TH codes that are either one dimensional system codes or multidimensional sub-channel codes and computational fluid dynamics (CFD) codes. Some of these involve TRACE [13], FLICA-4 [14], SUBCHANFLOW [15], Neptune-CFD [16] and RIGEL[12]. Therefore, as a result of the coupling of new coupled frameworks were born such as DYNSUB [17], POLCA-T [18], COBAYA3-SUBCHANFLOW [19], etc... among others. The need to couple these systems is a fact, as mention in the previous section. However, a clear idea for this need is shown in the N and TH equations. In the TH side the codes mentioned hereafter aim for solving the fluid field equations related the the conservation of mass, momentum and energy, in addition to the heat transfer, as described in the following equations:

$$\frac{\partial \rho}{\partial t} + \vec{\bigtriangledown} \cdot (\rho \vec{V}) = 0, \tag{1}$$

$$\frac{\partial \rho \vec{V}}{\partial t} + \vec{\bigtriangledown} \cdot (\rho \vec{V} \otimes \vec{V}) = \vec{\bigtriangledown} \bar{\bar{\tau}} - \vec{\bigtriangledown} P + \rho \vec{g}, \tag{2}$$

$$\frac{\partial \rho U}{\partial t} + \vec{\bigtriangledown} \cdot (\rho \vec{V} U) = -\vec{\bigtriangledown} q'', \tag{3}$$

$$\rho C_p \frac{\partial T}{\partial t} - \vec{\bigtriangledown} \cdot (k_f(T) \vec{\bigtriangledown} T) = q'''. \tag{4}$$

On the other side, the N codes mentioned in the following sections aim for solving the neutron diffusion approximation as represented in the following equations.

$$\frac{1}{v_g} \frac{\partial \phi_g(r,t)}{\partial t} = D_g \frac{\partial^2 \phi_g(r,t)}{\partial r^2} - \Sigma_{T,g}(T)\phi_g(r,t) - \sum_{g'>g}^{G} \Sigma_{s,g'->g}(T)\phi_{g'}(r,t) + \sum_{g'=1}^{G} \chi_g \nu \Sigma_{f,g'}(T)(1-\beta)\phi_{g'}(r,t) + \sum_{i=1}^{I} \chi_{g,i} \lambda_i C_i(r,t). \tag{5}$$

$$\frac{\partial C_i(r,t)}{\partial t} = \beta_i \sum_{g=1}^{G} \nu \Sigma_{f,g} \phi_g(r,t) - \lambda_i C_i(r,t), i = 1, 2, ..., I \tag{6}$$

A strong coupling between equations 1, 2, 3, 4, 5 and 6 is expected mainly through the temperature dependence of the cross-sections and the TH dependence on the heat generated by fission. Description of the terms in the previous equations are given at the end of the next sections. In these sections, some of the most known codes for TH and N analysis are described. This description is brief, with the objective of giving the generalities of the code. The definition of the equations mentioned hereafter are given in their respective reference.

## 3.1 Stand alone calculations

### 3.1.1 Thermal-hydraulic codes

**ATHLET** [20]:

The Analysis of THermal-hydraulics of Leaks and Transients (ATHLET) is being developed for the analysis of anticipated transients and abnormal plant transients, small and intermediate leaks, and large breaks in LWRs. The basic fluid-dynamic option is a five-equation model with individual conservation equations for liquid/vapor, mass and energy, a mixture momentum equation that accounts for thermal and mechanical non-equilibrium and which includes a mixture level capability. The time integration of the thermo-fluid-dynamics is performed with the general purpose ordinary differential equation solver called FEBE (Forward-Euler, Backward-Euler). It provides the solution of a general non-linear system of differential equations of first order, splitting it into two subsystems, the first being integrated explicitly (Forward-Euler), and the second implicitly (Backward-Euler). Generally, the fully implicit option is used. These explicit and implicit types of discretization are mentioned hereafter. Considering equation 7 and its discretization as equation 8.

$$\dot{x} = f(x,t), \tag{7}$$

$$\dot{x_n} = f(x_n,t_n). \tag{8}$$

By approximating the derivative and substituting into 7, one can obtain the explicit formulation (which applies for every type of first order systems) such as:

$$\frac{x_{n+1}-x_n}{\Delta t} = f(x_n,t_n), \tag{9}$$

$$x_{n+1} = x_n + \Delta t f(x_n,t_n). \tag{10}$$

In the implicit approach, this formulation has the form of:

$$\frac{x_n-x_{n-1}}{\Delta t} = f(x_n,t_n), \tag{11}$$

$$x_n = x_{n-1} + \Delta t f(x_n,t_n) \rightarrow x_{n+1} = x_n + \Delta t f(x_{n+1},t_{n+1}). \tag{12}$$

Since the term $x_{n+1}$ appears on both sides of equation 12, it is say to be implicit in $x_{n+1}$. Most of the time this requires a unique solution technique to solve for $x_{n+1}$ at each time step, so computationally speaking this is more expensive than the explicit method but has the advantage of being stable (unconditionally stable).

**CATHARE** [21] [22]:

CATHARE was directly developed for PWR plants, though it has recently been applied to the analysis of transients in VVERs and BWRs NPPs. All the CATHARE modules (except the 3-D module which is semi-implicit in time) use a fully implicit time discretization, both mentioned earlier in this section and which ensures the stability of the solution over a broad range of time step values. The TH of CATHARE is based on a 2 fluid 6 equation model: non condensible gases or radio-chemical components can be also modeled. The six main independent variables are pressure, liquid enthalpy, gas enthalpy, void fraction, liquid velocity and gas velocity. Inter-phase exchanges, pressure propagation and advective terms are thus totally implicitly evaluated. This numerical choice was made and implemented into CATHARE (developed in 1979), which main purpose was to reach the largest possible time step without time step limitation,

especially for transients of long duration. Concerning spatial nodalization, 1-D and 3-D modules use finite-volumes (FV)[1] discretization methods for mass and energy equations and finite-differences (FD) discretization methods for momentum balance equations. The meshes are staggered according to the Implicit Continuous-fluid Eulerian (ICE) method [23], where scalar points are bounded by vector points, mass and energy balances are assessed on scalar points and momentum balances are assessed on vector points. For transients, at each time step, it is necessary to find the solution of a set of non-linear equations; at which a full Newton iterative method is used.

**COBRA-III** [24] (one among the large family of COBRA codes):

COBRA-III is a code for TH calculations with implicit cross flows and homogeneous two phase fluids. It is used world-wide for DNBR analysis of LWR sub-channels, as well as for 3D whole PWR core simulation with one or more channels per fuel assembly. COBRA-III uses direct inversion at each plane for the axial flow equations with cross flows updated over an outer iteration loop, for the homogeneous model single phase coolant, and finite-element (FE) [2] direct solution for the fuel rod radial temperatures. FD are used in addition to a Successive-Over-Relaxation (SOR) and a Newton method to solve the system of equations. The equations that this code solves for two phase flow are the following [25]:

Conservation of mass:

$$A_i \frac{\partial \rho_i}{\partial t} + \frac{\partial m_i}{\partial x} = -\sum_{j=1} w_{ij}. \tag{13}$$

Conservation of energy:

$$A_i \frac{\partial \rho_i h_i}{\partial t} + \frac{\partial m_i h_i}{\partial x} = q_i' + \sum_{j=1}(h_i - h_j) w_{ij}' - \sum_{j=1} w_{ij} h *. \tag{14}$$

Conservation of lateral momentum:

$$\frac{\partial w_{ij}}{\partial t} + \frac{\partial w_{ij} u*}{\partial x} = \frac{s}{l}(p_i - p_j) - F_{ij}. \tag{15}$$

Conservation of momentum:

$$\frac{\partial m_i}{\partial t} + \frac{\partial m_i u_i}{\partial x} + \sum_{j=1}^{M}(u_i - u_j) w_{ij}' + \sum_{j=1}^{M} w_{ij} u* = -F_i - A_i \rho_i g cos\theta - A_i \frac{\partial \rho_i}{x}. \tag{16}$$

**FLICA4** [14]:

The French TH code FLICA4 is a 3D sub-channel code based on four equations plus two closure laws model. The code's drift-flux model (called Homogeneous Relaxation Model - HRM)[26] has been implemented on the basis of the Homogeneous Equilibrium Model (HEM). Its space time averaged local instantaneous equations work for structured and unstructured meshes. It provides a low diffusive method based on a fully implicit second order conservative scheme. As mentioned, the two phase flow model is based on four balance equations[3] , 17 to 20 (which are solved using a FV numerical scheme): three for the mixture and a mass balance equation for the less concentrate phase which permits the calculation of non-equilibrium flows as sub-cooled boiling and superheated steam [27].

$$\frac{\partial}{\partial t}\sum \alpha_k \rho_k + \nabla \sum (\alpha_k \rho_k u_k) = 0, \tag{17}$$

[1]Similar to the FDM, values are calculated at discrete places on a mesh at which volume integrals in Partial Differential Equations (PDEs) that contain divergence terms are converted to surface integrals by the divergence theorem.

[2]Method which consists on the assumption of piecewise continuous functions for the solution and obtain the desired parameter of the functions in a way that the error in the solution is minimized.

[3]More details on these equations are given in [27].

$$\frac{\partial}{\partial t}\alpha_k\rho_k + \nabla(\alpha_k\rho_k u_k + \alpha_k M_k) = \Gamma_{k'k} + \Gamma_{wk}, \tag{18}$$

$$\frac{\partial}{\partial t}\sum \alpha_k\rho_k u_k + \nabla\sum(\alpha_k\rho_k u_k \otimes u_k + \alpha_k\Pi_k) = \sum \alpha_k\rho_k g - \tau_w, \tag{19}$$

$$\frac{\partial}{\partial t}\sum \alpha_k\rho_k u_k E_k + \nabla\sum(\alpha_k\rho_k u_k H_k + \alpha_k Q_k) = \sum \alpha_k\rho_k g u_k + q + q_w. \tag{20}$$

The meshing is regular in the axial direction and triangular, quadrangular or hexagonal in the radial plane. A fully implicit second order numerical method is used to discretize the balance equations.

**FLOCAL** [9]:

FLOCAL is the 1D TH module of DYN3D[4]. It consists of a two phase flow model describing coolant behavior (including boron dilution transients) and a fuel rod model. The fuel elements are simulated by separate and parallel coolant channels. This channels are coupled hydraulically by the condition of equal pressure drop over all the channels. Additionally, some hot channels with power peaking factors belonging to chosen fuel elements can be described. The flow model is based on four differential balance equations for mass, energy and momentum of the mixture and mass balance of the vapor phase, at which water and steam properties are obtained from the IFC-67 and IAPWS-IF97 tables. A FV approach is used for their discretization. This TH model is closed by constitutive relations for the slip ratio, one and two phase frictional pressure losses, evaporation and condensation rates, heat transfer correlations and thermo-physical properties of the phases. The equation set that FLOCAL consider is presented hereafter [9]:

Mass balance of the mixture:

$$\frac{\partial[\phi\rho_v + (1-\phi)\rho_l]}{\partial t} + \frac{\partial[\phi\rho_v u_v + (1-\phi)\rho_l u_l]}{\partial z} = 0. \tag{21}$$

Mass balance of the vapor:

$$\frac{\partial\phi\rho_v}{\partial t} + \frac{\partial\phi\rho_v u_v}{\partial z} = \mu. \tag{22}$$

Momentum balance of the mixture:

$$\frac{\partial[\phi\rho_v u_v + (1-\phi)\rho_l u_l]}{\partial t} + \frac{\partial[\phi\rho_v u_v^2 + (1-\phi)\rho_l u_l^2]}{\partial z} + \frac{\partial P_{fric}}{\partial z} + \tag{23}$$

$g[\phi\rho_v + (1-\phi)\rho_l] + \frac{\partial P}{z} = 0.$

Energy balance of the mixture:

$$\frac{\partial[\phi\rho_v h_v + (1-\phi)\rho_l h_l]}{\partial t} + \frac{\partial[\phi\rho_v h_v + (1-\phi)\rho_l h_l]}{\partial z} = Q. \tag{24}$$

Mass balance of boron:

$$\frac{\partial\phi\rho_l c_b}{\partial t} + \frac{\partial u_l(1-\phi)\rho_l c_b}{\partial z} = Q. \tag{25}$$

The 1D heat conduction:

$$\rho C\frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial(\lambda r\frac{\partial T}{r})}{\partial r} + q'''. \tag{26}$$

[4]This code will be presented in the neutronic section in addition to the coupled scheme, which is presented in the coupled calculation section.

**POLCA-T(TH)** [12]: The TH is based on the RIGEL code.

RIGEL is the TH code that POLCA-T is based on, which model consists of a two fluid approach. The energy and mass are solved for both the liquid and vapor phases that may be in thermal non-equilibrium where the momentum is solved using a mixture model. Hence, POLCA-T is based on a five equation, 1D TH approach. The two FD mass conservation equations are coupled through phase change rates and the two FD discretized energy equations are coupled through inter facial heat transfer models. The FD formulation of the 1D momentum equation considers pressure losses in both phases. The main features of this code are mentioned hereafter.

1. Thermal non-equilibrium, i.e. two fluid model (mixed momentum).
2. None condensible gases and boron transport.
3. Heat conduction in different geometries (FD).
4. Advanced fuel rod calculation, gas gap heat transfer coefficient, rupture and creeping.

In addition, several constitutive relationships based on empirical correlations that model inter facial and wall phenomena are used to close the TH model. The interfacial heat and mass transfer are treated in two components. The first component addresses heat and mass transfer between the phases and the heated wall boundary, and the second component addresses heat and mass transfer within the bulk of the fluid. Pressure drops are calculated for each phase in the two fluid model and therefore, the total pressure drop across a given node is the sum of the pressure loss in the vapor and liquid phases. The slab and cylindrical heat conduction models are based on a time-discretized analytical solution of the heat conduction equation. The implicitness factor is set to 1/2, also referred as the Crank-Nicholson method. This type of discretization is a FD method used for solving PDEs which involves a central difference in time and second-order central difference in space, which recurrence relation for $x_t = x_{zz}$ is given by:

$$\frac{x_z^{t+1} - x_z^t}{\Delta t} = \frac{1}{2}\left(\frac{x_{z+1}^{t+1} - 2x_z^{t+1} + x_{z-1}^{t+1}}{\Delta z^2} + \frac{x_{z+1}^{t} - 2x_z^{t} + x_{z-1}^{t}}{\Delta z^2}\right). \tag{27}$$

**RELAP5** [28]:

RELAP5 is a TH system code extensively used for the analysis of any kind of transients in LWRs. The code is based upon the solution of six PDEs that are coupled. The numerical solution method is based upon the use of a semi-implicit FD [5] technique. Another possibility is to choose a more stable but diffusive nearly implicit scheme. This scheme has the convective fluxes evaluated implicitly, and hence eliminates the material Courant time step stability restriction. This technique is derived from the fact that implicit schemes can often be converted to explicit schemes by limiting the number of iterations used to solve the implicitness. In addition, the methods are called semi-implicit since the right hand side of the schemes involve approximations at the current state level "$n$" and at the previous stage, "$n-1$", as shown next and based on equation 8.

$$\frac{x_n - x_{n-1}}{\Delta t} = f(x_n, t_{n-1}), \tag{28}$$

The code is capable of modeling the primary and secondary circuits (where applicable) of NPPs as well as all the components belonging to the balance-of-plant[6].

**SUBCHANFLOW** [15] [29]:

SUBCHANFLOW is a computer code used to analyze TH phenomena in the core of PWRs, BWRs, and innovative reactors operated with gas or liquid metal as coolant. In SUBCHANFLOW, a three-equation two-phase flow model, that is a mixture equation for mass, momentum, and energy balance, is

[5] Finite-Difference Schemes (FDS) aim to solve differential equations by means of finite differences.

[6] These components consists on the remaining systems, and structures that include a complete nuclear power plant and are not included in the nuclear steam supply system.

implemented. The constitutive relations are expressed as mixture equations for wall friction and wall heat flux as well as a slip velocity relation. In addition, user defined empirical correlations can be implemented. The solution method is repeated several times during each time step resulting in a fully implicit scheme. For steady-state calculations, the time step is set to a very large value. The sketched solution algorithm is limited to cases with axial flow rates which are always kept positive (up flow). The fuel rod or heater rod temperatures are calculated in each iteration step depending on power release and cladding to coolant heat transfer. The linear equation system built up by the energy equations in each layer is solved by the SOR method (the equation system for the pressure gradients can be also solved by a direct scheme) which needs much less memory storage. This method represents a variation of the Gauss-Seidel method for solving linear system of equations. In general, the over-relaxation method ($w > 1$) involve:

$$x_i^k = x_i^{k-1} + w\frac{r_{ii}^k}{a_{ii}}, \tag{29}$$

where "$r$" is the residual vector with respect to "$r = b - Ax$" and "$a$" is the component of the matrix associated to "$A$", if the solution of the system is represented by "$Ax = b$". In fact, when SUBCHANFLOW solves the matrices through this method, the matrix "$A$" is decomposed into a diagonal (D), lower triangular (L) and upper triangular (U) such as: $Ax = b$, where, $A = D + L + U$. This SOR iterative process solves "$x$" using its previous value.

**TRACE** [30]:

TRACE is the best-estimate code developed by the US NRC for analyzing 1D/3D steady states and transients of LWRs. The TH involves a six equations model following a FV discretization and is able to analyze LOCAs and general transients on PWRs and BWRs. The energy equation is solved using a semi-implicit scheme and the fluid motion using a stability-enhancing two-step (SETS)[7] numerical model. In addition, one could also choose a semi-implicit scheme with possible $2^{nd}$ order with flux limiter schemes. When SETS is used (default option in TRACE), the method solves first the stabilizer momentum equation, then solve all other equations except energy and mass, and finally the energy and mass equations for the new time step. The field equations that TRACE solves are presented hereafter, which details are given in the TRACE manual [31] and [32].

Mass:

$$\frac{\partial}{\partial t}\sum \alpha\rho_g + \nabla\cdot[\alpha\rho_g\vec{V}_k] = \Gamma, \tag{30}$$

$$\frac{\partial((1-\alpha)\rho_l + \alpha\rho_g)}{\partial t} + \nabla\cdot[(1-\alpha)\rho_l\vec{V}_k + \alpha\rho_g\vec{V}_g] = 0. \tag{31}$$

Momentum:

$$\frac{\partial\vec{V}_l}{\partial t} + \vec{V}_l\cdot\nabla\vec{V}_l = -\frac{1}{\rho_l}\nabla P + \frac{f_i - \Gamma(\vec{V}_i - \vec{V}_l) + f_{wl}}{(1-\alpha)\rho_l} + \vec{g}, \tag{32}$$

$$\frac{\partial\vec{V}_g}{\partial t} + \vec{V}_g\cdot\nabla\vec{V}_g = -\frac{1}{\rho_g}\nabla P + \frac{f_{wg} - f_i - \Gamma(\vec{V}_g - \vec{V}_i) + f_{wl}}{(1-\alpha)\rho_g} + \vec{g}. \tag{33}$$

Internal Energy:

$$\frac{\partial\alpha\rho_g e_g}{\partial t} + \nabla\cdot(\alpha\rho_g e_g\vec{V}_g) = -P\frac{\partial\alpha}{\partial t} - P\nabla\cdot(\alpha\vec{V}_g) + q_{dg} + q_{ig} + \Gamma h_v', \tag{34}$$

$$\frac{\partial(1-\alpha)\rho_l e_l + \alpha\rho_g e_g}{\partial t} + \nabla\cdot((1-\alpha)\rho_g e_g\vec{V}_g + \alpha\rho_l e_l\vec{V}_l) = \tag{35}$$

$-P\nabla\cdot((1-\alpha)\vec{V}_l + \alpha\vec{V}_g) + q_{wl} + q_{wg} + q_{dg} + q_{dl}$.

[7] This scheme allows to exceed the Courant limit and therefore use longer time steps. This is done by applying a correction step on a semi-implicit scheme. However, the main disadvantage is its relative high numerical diffusion, which turns into a non-perfect conservation of mass in closed components.

### TRAC-BF1 and TRAC-PF1(J-TRAC) [33] [34]:

The Idaho National Engineering Laboratories in collaboration with General Electric developed the original TRAC TH family of codes in the mid 70's for the analysis of BWRs (-B series) [35] and PWRs (-P series)[36]. The code solves the general transient two-phase coolant conditions in one, two or three dimensions using a realistic six-equations, two-fluid, FD model combining 3D hydrodynamics and 1D balance-of-plant modeling. A two-dimensional treatment of fluid-wall heat transfer is incorporated through the ROD component. This component or module provides the treatment of power generation and its transfer to the coolant.

### VIPRE-02 [37]

The VIPRE-02 code employs a six equations model for solving fully implicitly the liquid and vapor fields. The HEM model can be used in 3D rod bundles at sub-channel level. The code is intended to perform steady state and transient simulations during normal and ab-normal conditions.

---

Notation in the general equations: 1 to 4 .

| Symbol | Definition |
|---|---|
| $\rho$ | Coolant density |
| $\vec{V}$ | Flow velocity |
| $\bar{\bar{\tau}}$ | Stress tensor |
| $P$ | Pressure |
| $U$ | Internal energy |
| $q''$ | Surface heat flux |
| $q'''$ | Volumetric heat flux |
| $C_p$ | Material specific heat |
| $k$ | Material thermal-conductivity |
| $T$ | Temperature |
| $\vec{g}$ | gravity |
| $t$ | time |

### 3.1.2 Neutronic codes - Core simulators

**ARROTTA** [38]:

ARROTTA (Advanced Rapid Reactor Operational Transient Analyzer) is a 3D space-time kinetic code used for solving LWRs transients with specific emphasis on spatial effects. ARROTTA neutronics uses the Analytical Nodal Method (ANM) combined with BiCGSTAB iterations to solve the system of equations. In ANMs, the solution of the 1D diffusion equation in matrix form (equation 36) is obtained through trigonometric and hyperbolic functions.

$$D\frac{d^2}{df^2}\Phi_f(f) = A\Phi_f(f) + B_u(f). \tag{36}$$

**BIPR8NK** [39]:

The code BIPR8NK [39] uses the two group 3D hexagonal coarse mesh nodal approximation for the neutron flux. The kinetic branch of the code calculates the core power and the 3D neutron flux deformation as a function of time, caused by reactivity perturbations of different natures taking into account prompt neutrons, six delayed neutron groups and feedback effects.

**COBAYA3** [10] [25] [40]:

The code has been designed to provide computational tools needed for core calculation at both nodal and pin levels. The solution method for kinetics calculations is based on a scheme with an implicit time step discretization both for the diffusion and the delayed neutron equation. The code also includes subroutines of the mathematical libraries LAPACK, SPARSKIT and HIPS to solve the system of linear equations by direct or iterative methods. In addition, the iterative solvers that have been implemented are namely, the relaxed Gauss-Seidel, BiGGSTAB and GMRES methods. For the nodal solver (ANDES), the exponential extrapolation method has been implemented to permit the increase of the time step when the core N conditions evolve slowly. It solves the multi-group 3D diffusion equation based on the Analytical Coarse Mesh Finite Difference Method (ACMFDM)[41]. For the steady state solution, ANDES employs a power iteration method for calculating the Eigenvalue through [42]:

$$FM^{-1}|S_{n,g}>= k_{eff}|S_{n,g}. \tag{37}$$

For the pin by pin solver (COBAYA3k) both and Euler and a Crank-Nicholson discretization have been implemented to allow larger time steps. The multi-group 3D diffusion equation is solved on fine meshes using the technique of alternate dissections, which consists in dividing the geometry in sub-domains in the radial direction so that each sub-domain represents a closed problem leading to individual solutions. NEMTAB tabulated cross sections are needed in advance to perform the N solution. This homogenized cross section format implies an a-priori lattice calculation to obtain the temperature, density, boron and void dependences of the cross sections, which are tabulated and cover a large range of core operating conditions. This type of format is widely used by core simulators. A sample of a two groups cross section NEMTAB format is shown in figure 2, where only the cross sections related to one material type and one burn-up point are shown.

Figure 2: Example of a 2 groups tabulated cross section in NEMTAB format [43].

```
*   Mod Dens    Boron ppm    Fuel Temp     Mod Temp
      3           3       3        0
     661.14       711.87      752.06
      0.00      1000.00     2000.00
     560.00       900.00     1320.00
*
* ---------------------------------------------------------
* BURNUP  0.15
* ---------------------------------------------------------
*
* Transport XSEC Table
*
* GROUP    1
  XS(D1,B1,F1)  XS(D2,B1,F1)  XS(D3,B1,F1)
  XS(D1,B2,F1)  XS(D2,B2,F1)  XS(D3,B2,F1)
  XS(D1,B3,F1)  XS(D2,B3,F1)  XS(D3,B3,F1)
  XS(D1,B1,F2)  XS(D2,B1,F2)  XS(D3,B1,F2)
  XS(D1,B2,F2)  XS(D2,B2,F2)  XS(D3,B2,F2)
  XS(D1,B3,F2)  XS(D2,B3,F2)  XS(D3,B3,F2)
  XS(D1,B1,F3)  XS(D2,B1,F3)  XS(D3,B1,F3)
  XS(D1,B2,F3)  XS(D2,B2,F3)  XS(D3,B2,F3)
  XS(D1,B3,F3)  XS(D2,B3,F3)  XS(D3,B3,F3)
* GROUP    2
  ...
*
* Absorption XSEC Table
  ...
*
* Nu-Fission XSEC Table
  ...
*
* Kappa-Fission XSEC Table
  ...
*
* Scattering XSEC Table
*
* GROUP    1 ->      2
  ...
* GROUP    2 ->      1
  ...
*
* ADF Table
  ...
*
* Fission Spectrum
*
* GROUP    1       2
    CHI(G1)    CHI(G2)
*
* Inverse Velocity
*
* GROUP    1       2
    IVEL(G1)    IVEL(G2)
*
* Delay Neutron Decay Constant (Lambda)
*
* GROUP    1       2       3       4       5       6
```

**COS3D** [44]:

The code COS3D is mainly a BWR core simulator based on the 1D, one group diffusion theory. In addition, and as a response of the simplified 1D neutronics, it has been improved by using few groups nodal expansion methods with flux discontinuity factors between fuel assemblies.

**CRONOS2** [45]:

CRONOS2 is a 3D N code used for core calculations based on the solution of diffusion or transport, with focus on dynamical or static equations. Its two main flux solvers are: PRIAM, based on an even parity formulation using a FE approximation in space and a SN discrete ordinate in angle, and MINOS, which uses a powerful nodal method for dealing with structured geometries. The resolution method for kinetic calculations is based on a scheme with an implicit time step theta method (which regulates the implicitness of the system). The delayed neutron equations are integrated exactly.

**DYN3D** [46]:

The code DYN3D is adequate to investigate reactivity transients in the cores of thermal power reactors with hexagonal or quadratic fuel assemblies. The 3D neutron kinetic model is based on the Nodal Expansion Method (NEM) for solving the two group diffusion equation, which nodes are coupled by the side averaged values of the neutron flux and currents. The neutron group constants are assumed to be spatially constant in each node and the solving of the time dependent (implicit scheme) neutron diffusion equation, including delayed neutrons for all nodes, is used for transient calculation. The NEM method in cartesian geometries is based on the transverse integration over all the combinations of two directions on rectangular nodes[9], leading to 1D equation for all directions. Considering one direction in "$x$", the transverse integration over "$y$" and "$z$" leads to:

$$-D_g \frac{d^2\Phi_g(x)}{dx^2} + \Sigma_g \Phi_g(x) = Q_g(x), \tag{38}$$

where "$Q$" depends on the transverse integrated leakage term. In fact, while applying the NEM to 38, the solution is approximated by an expression of known functions based on expansion coefficients.

**ENTRÉE** [47]:

ENTRÉE is the BWR core analyzer that solves the two energy groups 3D diffusion equation by applying the transverse integrated NEM. The bundle flux is expanded with Legendre (polynomial or semi-analytical) functions. ENTRÉE introduced an efficient pin power reconstruction method based on the average of the fluxes to limit the constraints provided by the homogenized power shape.

**KIKO3D** [48]:

KIKO3D is a 3D code that discretizes the core using sub-divided nodes. Six delay neutron groups are considered, while the neutron balance equation has the form:

$$T(r,t)\Psi(r,t) = (\frac{1}{v}\frac{\partial(-\chi\beta F(r,t))}{\partial t})\Psi(r,t) + \chi\sum_{j=1}\lambda_j C_j(r,t), \tag{39}$$

and the precursor concentration,

$$\frac{dC(r,t)}{dt} = -\lambda_j C_j(r,t) + \beta_j F(r,t)\Psi(r,t). \tag{40}$$

Where "$F(r,t)$" is the fission operator, "$\Psi(r,t)$" the two groups scalar flux, "$\beta$" the delay neutron fraction, "$C_j(r,t)$" the precursor density and "$\chi$" the fission spectrum. For the numerical solution of the point kinetics, KIKO3D uses Runge-Kutta methods. For solving the large and sparse equation system derived from discretizing equations 39 and 40, the code uses the GMRES and BiCGSTAB algorithms.

**NEM** [49]:

NEM is a 3D multi-group code used for modeling both steady state and transient core conditions for cartesian, cylindrical and hexagonal geometries. Its source is the NEM for solving the nodal equations in 3D. This methodology (which traditionally uses the "red-black" scheme related to the Parallel SOR method) has as objective, to obtain the nodal average flux by solving the nodal balance equation [50]:

$$\sum_{u=x,y,z}\frac{1}{2\Delta_u^k}[J_{gu+}^k - J_{gu-}^k] + \Sigma_g^{r,k}\phi_g^k = Q_g^k. \tag{41}$$

However, a transverse integration strategy is used to obtain 1D transverse integration equations and obtain the relationships between surface average net currents and average flux within the node, which is needed

to solve equation 41. NEM assumes that the 1D integrated flux in each node can be approximated by an expansion of known functions such as:

$$\phi_{gx}^{k} = a_{gx}^{k} + \sum_{n=1} a_{gxn}^{k} f_{n}^{k}(r). \tag{42}$$

By substituting equation 41 into Flick's law, a response matrix equation is obtained, which combined with equation 42 and applying a standard source iteration method, a solution for the flux distribution and the eigenvalue is obtained. The nodal coupling relationships are expressed in partial current formulation and the time dependence of the neutron flux is approximated by a 1st order fully explicit, FD scheme.

**NESTLE** [51]:

NESTLE is a multi-dimensional neutron kinetics code which solves the two or four groups diffusion equations in cartesian or hexagonal geometries using the NEM and the non-linear iteration technique. The steady state eigenvalue and time dependent neutron flux problems can be solved. The new Border Profile Lower Upper matrix solver (BPLU, also implemented in the TH code RELAP5) is used to efficiently solve sparse linear systems. The BiCGSTAB algorithm is also used to solve the system and a FE discretization method is employed.

**PANBOX** [52]:

The standard PANBOX model includes a 3D diffusion based neutronic solution, however a 1D and point kinetics model are also available in the code. It is a nodal space-time kinetic core model capable of solving transients using both the polynomial and semi-analytical nodal expansion methods (SANEM). The code presents an adaptive algorithm that switches dynamically the 3D, 1D or 0D solutions during transient investigations. The criteria for this switch is based on the monitoring of the time derivative $\frac{\partial \chi_g^{1D}(t)}{\partial t}$ during original 3D calculations.

**PANTHER** [53]:

The code PANTHER provides a relatively easy and quick reference for PWR calculations. Nevertheless, it has been tested for different BWRs, VVERs and research reactors using the NEM. It solves implicitly the multi-group homogeneous neutron diffusion equation in steady state and transient situations (for 0D, 1D, 2D and 3D).

**PARCS** [11]:

PARCS is a 3D reactor core simulator that solves the steady state and time dependent two groups neutron diffusion equation to predict the dynamic response of the reactor to reactivity perturbations. The coarse mesh finite difference (CMFD) formulation is employed to solve the neutron fluxes in homogenized nodes. The temporal discretization is performed using the theta method with an exponential transformation of the group fluxes along with a second order analytic precursor integration technique. A transient fixed source problem is formed and solved at each time point in the transient. The solution of the CMFD linear system is obtained using a Krylov subspace method that employs the BILU3D pre-conditioner in rectangular geometries and a point pre-conditioner in hexagonal geometries[8]. In the CMFD formulation, the reactor core is discretized into coarse meshes (fuel assembly size,≈20cmX20cm) and finite differences are applied between nodes. Moreover, the eigenvalue problem is solved [9] through the fission source

[8]This Krylov method and pre-conditioning is discussed in the report devoted to task 1b of the X-TREAM project.

[9]Details about this procedure are given in [54] in addition to the full theory behind the CMFD method.

iteration method applied to:

$$M\phi^{n+1} = s^n = \frac{1}{k_{eff}} F\phi^n. \tag{43}$$

To accelerate this iteration method, PARCS uses a Wielandt shift (also used in COBAYA3). Its effectiveness depends on the shift $\delta k$ applied to $k_s^n = k_{eff}^n + \delta k$ in:

$$(M - \frac{1}{k_s^n} F)\phi^{n+1} = s^n = (\frac{1}{k_{eff}} - \frac{1}{k_s})F\phi^n. \tag{44}$$

**POLCA7** [12] [55]: The N is based on the POLCA7 code.

The FORTRAN 95 POLCA7 code, which implements dynamic memory allocation, is a 3D nodal diffusion 2 groups neutronic code used to predict the reactivity, nodal power and pin power distribution of reactor cores. The code uses the analytical nodal method for predicting steady states with Assembly Discontinuity Factors (ADF). The POLCA7 models involve:

- Pin power reconstruction model.
- Detector models.
- Thermal loads and margins calculations.
- Nodal models: The NEU3, a standard 2-groups Analytic Nodal Method (ANM) with quadratic transverse leakage approximation. This is the default method used for both BWRs and PWRs.
- Iteration schemes for solving the system of equations.
- Axial homogenization model.
- Reflector model.
- Cross section model.
- Depletion models.

Roughly speaking, the ANM mentioned in the previous list combines the attractive features of the FEM and the FDM. Through the FEM, the unknown function is approximated over a coarse mesh by continuous functions [56]. Through the FDM, the system of algebraic equations are sparse and well structured because the parameters are cell and edge values of the unknown functions, which connect at most, two adjacent nodes. POLCA7 receives the nuclear parameter input from the upstream 2D lattice-physics and global diffusion code PHOENIX. This last code generates cross section data taking into account fuel exposure, coolant density and instantaneous dependencies, control rods, spacer grids, fuel temperature, and xenon dependencies. The spectral history is specifically accounted by solving depletion chains for heavy nuclides and fission products. This treatment allows a substantially more accurate treatment of spectral and burn-up effects. The fission power calculated by POLCA7 is divided into two parts, the part deposited directly in the coolant (direct moderator heat), and the heat deposited in the fuel rods. The code calculates the prompt and delayed neutrons, in addition to decay power derived from the American Nuclear Society Standard 5.1 or by user supplied data. The axial homogenization model uses a 1D diffusion solver to determine axial discontinuity factors to calculate nodal parameters with varying axial geometry (such as control blade insertion).

**QUABOX-CUBBOX** [57] [58]:

In QUABOX the neutron flux is approximated within the nodes by the sum of 1D Taylor polynomials. This neutron kinetics code is suited for 3D core neutron flux and power calculations in steady state and transient conditions solving the two group energy diffusion equation through local polynomial approximation. For CUBBOX higher approximations (cubic) are used, but the set of admissible functions requires additional conditions. Some variational methods that have been proposed use spline functions and Galerkin weighting (weighted residual method).

**SIMULA-3** [59]:

SIMULA-3 uses the two group 3D nodal theory (including a six-group model for delayed neutron precursors) with a transport kernel to provide the same node interface leakages than a fine mesh diffusion calculation. Its numerical solution involves a SANEM. Radial and axial reflectors are replaced by albedo factors, so only regions within the active fuel region are taken into account. Its physical models include source or power iteration methods, criticality search and fuel burn-up.

**SIMULATE-3K(solid foundation of SIMULATE3)** [60],[61]:

SIMULATE-3K solves the neutron diffusion equations in one or two groups, on 3D coarse mesh nodes. This is done by using a linear discontinuous FD scheme where the interface net currents are given in terms of the actual node average and the corrected interface averaged fluxes using a synthetic interface flux discontinuity factors for each group and node interface. The code solves the nodal diffusion problem in a 3D domain composed of core and reflector using the selected number of energy groups. In the calculation, the neutron flux is divided into fast energy and thermal energy groups. The intra nodal flux is calculated involving node average fluxes and transverse leakages by polynomial representations (of each group) treating two nodes simultaneously.

**SKETCH-N** [62]:

SKETCH-N solves the diffusion equation in 3D for steady state and kinetic problems, treating arbitrary number of neutron energy groups and delay neutron precursors. The spatial discretization is done through polynomial and SANM based on non-linear iteration procedures. A fully implicit scheme is used for the time integration with automatic time step characteristics.

---

Notation in the general equation 5 .

| Symbol | Definition |
|---|---|
| $\frac{1}{v_g}$ | Inverse neutron velocity |
| $\phi_g$ | Neutron flux related to group, $g$ |
| $D_g$ | Diffusion coefficient related to group, $g$ |
| $\Sigma_{T,g}$ | Transport cross section, group "g" |
| $\Sigma_{s,g'->g}$ | Scattering cross section from group $g$' to $g$ |
| $\chi_g$ | Fission spectrum |
| $\nu$ | Fission yield |
| $\Sigma_{f,g}$ | Fission cross section, group "g" |
| $\beta$ | Delay neutron fraction |
| $\chi_{g,i}$ | Delayed neutron spectrum |
| $\lambda_i$ | Delay neutron constant |
| $C_i$ | Delayed neutron concentration |
| $G$ | Total number of groups |
| $I$ | Total number of delayed groups |

## 3.2 Coupled calculations: Core-Simulators + Core-Thermal-Hydraulics

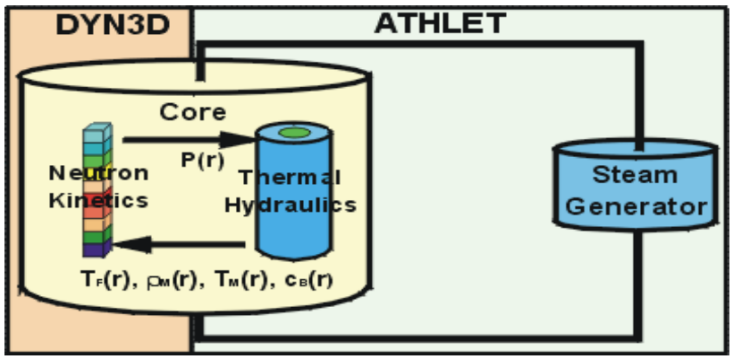
In this sub-section, some of the most common and used coupled codes are listed. A very general description is presented, emphasizing mostly the numerical methods. In addition, the numerical schemes commonly used in the nuclear engineering field are shown. Moreover, certain requirements with regard to the coupling of thermal-hydraulics and neutronics are considered. The objective of these requirements is to provide accurate solutions in a reasonable amount of CPU time in coupled simulations of detailed operational transients and accident scenarios. One of these requirements, and in fact the one that this report focuses on, is devoted to coupled algorithms and numerics. Many of the coupling efforts utilize simple code coupling or first order operator splitting schemes. They are often referred to as loose coupling. While these approaches can produce answers, they usually leave questions of accuracy and stability unanswered. Additionally, the different physics often reside on separate grids which are coupled via simple interpolation, again leaving open questions of stability and accuracy. In nuclear engineering (and due to the multi-physics problems involved) the choices of time integration and spatial discretization of the coupled system is a critical issue to consider. Usually, first order operator splitting or even explicit coupling of different codes is used to perform the time integration. A particular solution which could be the answer to the problems of accuracy and high computing costs in the calculations, is the usage of the so called Jacobian-Free Newton-Krylov (JFNK) method for solving the non-linear system of equations. This algorithm has many of the desirable features of operator splitting but can significantly reduce the time integration error and stability issues. The JFNK combined with physics based preconditioning is a modern multi-physics algorithm. Details about all the coupling schemes mentioned in the following sections are presented in the report devoted to the task 1b of the X-TREAM project.

### 3.2.1 Coupled codes

**ATHLET** - coupled with the N codes:
DYN3D [63] - BIPR8NK [64] - KIKO3D [48] [65] - (QUABOX/CUBBOX/TORT-TD) [66]:

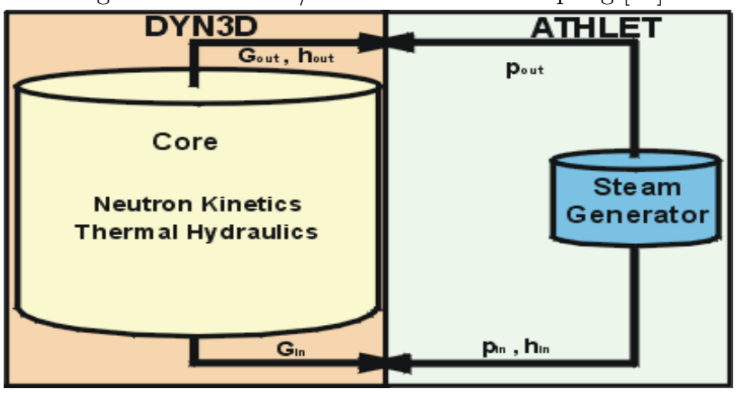
In this solution procedure (ATHLET/DYN3D), very tight coupling is achieved. The data must be exchanged between all core nodes of the single models (internal coupling), resulting in the transfer of a great number of data. In accomplishing the coupling of ATHLET and DYN3D three basically different ways were pursued. The first one uses only the neutron-kinetic part of DYN3D and couple it to the heat transfer and heat conduction model of ATHLET, where plant boundary conditions are also provided by the code. This is a very close coupling and the data have to be exchanged between all core nodes of the single models (internal coupling). Table 1 present the parameters seen in the following figures.

Figure 3: ATHLET/DYN3D internal coupling [67].



In the second type of coupling the whole core is cut out of the ATHLET plant solution and is completely modeled by DYN3D (external coupling), making use of its TH (FLOCAL) module.

Figure 4: ATHLET/DYN3D external coupling [67].




For the third type of coupling, the TH is split into two parts: the FLOCAL core model of DYN3D and the ATHLET model of the core and cooling system. Boundary conditions are provided to the DYN3D by the core TH solution of ATHLET.

Figure 5: ATHLET/DYN3D parallel coupling [67].

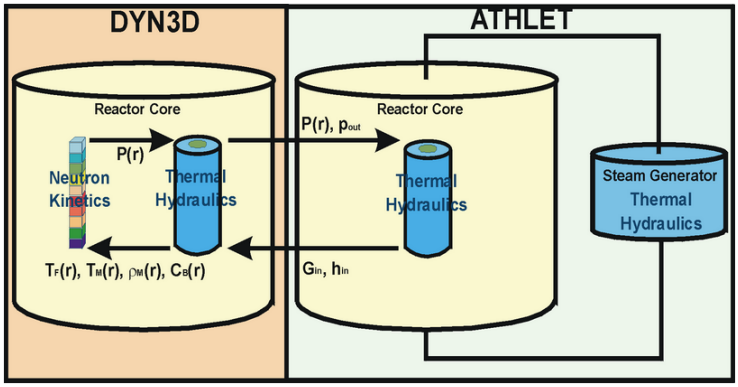



Table 1: Symbols in the previous figures 3 to 5.

| Symbol | Definition |
|---|---|
| P(r) | Thermal power |
| $T_F$(r) | Fuel temperature |
| $T_M$(r) | Moderator temperature |
| $\rho_m$(r) | Moderator density |
| $C_B$(r) | Boron concentration |
| $P_{out}$ | Outlet pressure |
| $P_{in}$ | Inlet pressure |
| $h_{out}$ | Outlet enthalpy |
| $h_{in}$ | Inlet enthalpy |
| $G_{out}$ | Outlet mass flow |
| $G_{in}$ | Inlet mass flow |

As a consequence of this local cut, it is easy to define the interfaces. They are located at the bottom and at the top of the core. The pressures, mass flow rates, enthalpies and concentrations of boric acid at these interfaces have to be transferred. So the external coupling needs only a few parameters to be exchanged between the codes and is therefore easy to be implemented. Recently, a third way of coupling has been developed. In this type parallel coupling is used: the core power is calculated by the neutron-kinetic part

of DYN3D and transferred to the core TH models of both ATHLET and DYN3D. This type of coupling has demonstrated its advantages in transients where very small time steps are necessary, which sometimes pose a problem in external-coupling calculations.

For ATHLET/BIPR8NK, the calculation of the initial stationary condition is made iteratively until all TH and neutron-kinetic parameters achieve stationary values. During the transient calculation, the so-called "close" connection of the codes is used, i.e. in case of BIPR8NK/ATHLET the joint solution of TH and neutron-physical parts of a problem is searched in explicit form. The core model is calculated at the end of each ATHLET time step. In each part of the coupled code (hydraulics, heat transfer, neutron kinetics) the maximal allowable time step for integration is estimated. The coupling methodology requires a parallel scheme, at which the core is modeled in the system code and in the core model, and the calculated reactor power is transferred to both models. The whole problem is solved with the minimum of the time steps in the separated modules. If the change of a parameter through a time step exceeds the given limiting value, the calculation of the actual time step is repeated, dividing it into a number of smaller time steps.

For ATHLET/KIKO3D, the coupling of 3D N models to the system code that models completely the TH in the primary circuit including the core region is achieved. In this case ATHLET obtains the heat source from the decay heat model of KIKO3D. The fuel and moderator temperatures, moderator densities and boron concentrations necessary for the feedback in KIKO3D originate from the ATHLET program. The drawback of this method is that the assumed discretization of the TH system code is too coarse to take into account the node-wise feedback effects.

In ATHLET/(QUABOX/CUBBOX/TORT-TD), using an internal coupling approach, QUABOX and CUBBOX provide the assembly-wise 3D power distribution and TORT-TD[10] provides the 3D pin power distribution. Thereafter, ATHLET calculates the TH through a single executable controlled by this last code. Time integration in the neutronics code QUABOX/CUBBOX is performed separately. Thus, both codes maintain their capabilities leading to an explicit type of coupling approach.

**Apros** [68] [69]:

Pros (Advanced Process Simulation environment) is a multi-functional software for simulation of industrial processes developed by VTT, the Technical Research Center of Finland. The system code Apros is well-suited for NPP transient analysis in benchmarking purposes. Apros includes a 1D and 3D core neutronic models, which uses a finite difference approximation model able to describe hexagonal and quadrilateral fuel assembly geometries. Both models have 2 energy groups and the 6 delayed neutron groups are calculated in each cell using a first order discretization for the time derivative. For the 3D model the equations are integrated over the node volumes and are solved using the Gauss-Seidel iteration process.

In the TH side, Apros includes the drift flux five equations and two phase flow six equations models limited to 1D TH flow channels (whole core capabilities). The six equations model solve quantities such as phase enthalpies and concentrations using second-order upwind schemes. This TH model allows the user to calculate fuel rod temperatures, coolant conditions and boric acid concentrations. The flow solution of Apros is based on the staggered grid discretization scheme. In this scheme the state variables such as pressure and enthalpy are calculated at the mesh center. The steam tables used in Apros are based on the IAPWS-IF97 recommendation. The physics are coupled through the traditional OS approach. Specific details about the N and TH can be found in [70] and [71] respectively.

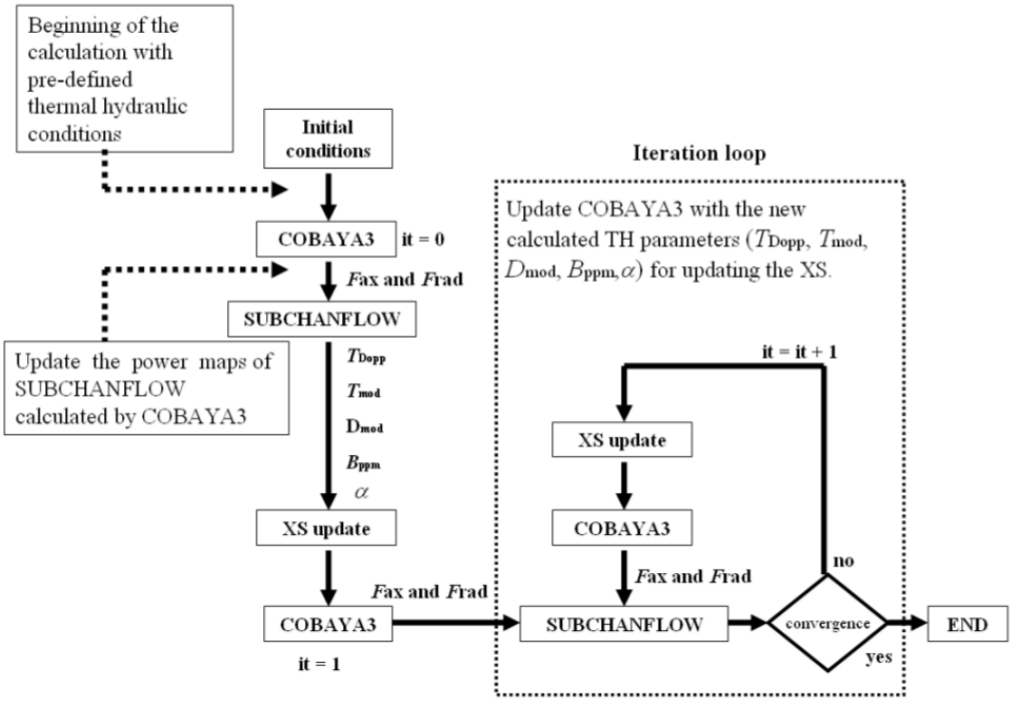
The validation of the code has been consistent and independent benchmarks have been modeled for the N and TH sections. However, special validation cases used regularly at each Apros version change involve the; LOVIISA NPP, VVER-400 NPP, Olkiluoto 1 NPP, Forsmark 3 NPP (HAMBO), LOVIISA ice condenser containment, and CCGT power plant model with district heating circuit.

**COBAYA3/SUBCHANFLOW** [72] [19]:

[10]TORT-TD is a time dependent 3D fine-mesh discrete ordinate Sn neutron transport code.

The coupling approach between the 3D neutron diffusion code COBAYA3 and the sub-channel code SUBCHANFLOW has been done within SALOME (an open source platform that is characterized by powerful pre- and post-processing capabilities and a novel functionality for mapping of the neutronic and thermal hydraulic domains) using the MED (Memory Exchange Data) format. The coupling has been done following an operator splitting approach at which the N is the master and the TH follows the N time step discretization. The mapping is done using independent meshes inside the simulation platform. In figure 6 the parameters $T_{Dopp}.T_{mod}, D_{mod}, B_{ppm}$ and $\alpha$ represent the Doppler temperature, moderator temperature and density, boron concentration and void fraction respectively. In the N side, $F_{ax}$ and $F_{rad}$ represent the axial and radial power factors respectively.

Figure 6: COBAYA3/SUBCHANFLOW: Explicit coupling scheme for the steady state solution [42].

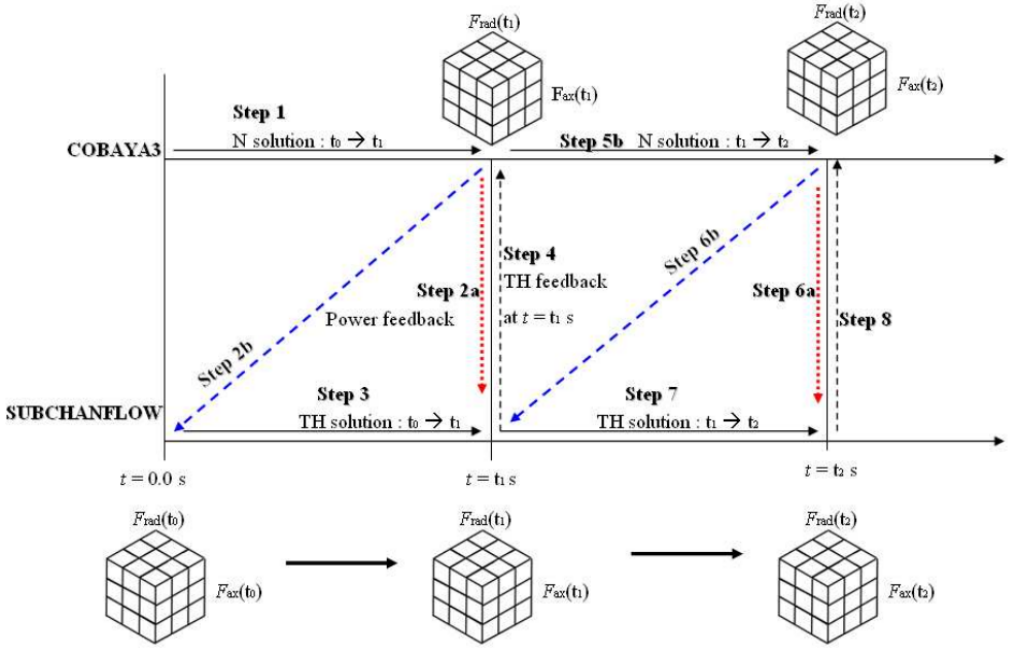



The convergence is checked through the simple formulation:

$$\frac{X^n - X^{n-1}}{X^n} = \epsilon(convergence - criteria), \tag{45}$$

where $X = T_{Dopp}, D_{mod}, Pow_{tot}$ and $K_{eff}$. Moreover, figure 7 illustrates the temporal coupling between COBAYA3 and SUBCHANFLOW.

Figure 7: COBAYA3/SUBCHANFLOW: Coupling scheme for the time dependent solution [42].




In the previous figure the red arrow represents the N to TH power feedback at the current time step, and the blue arrow the sequence or code that follows the solution. In other words, after Step 1 (pure N) is completed, the code that will be executed next is SUBCHANFLOW. This change of solver is illustrated by the blue arrow.

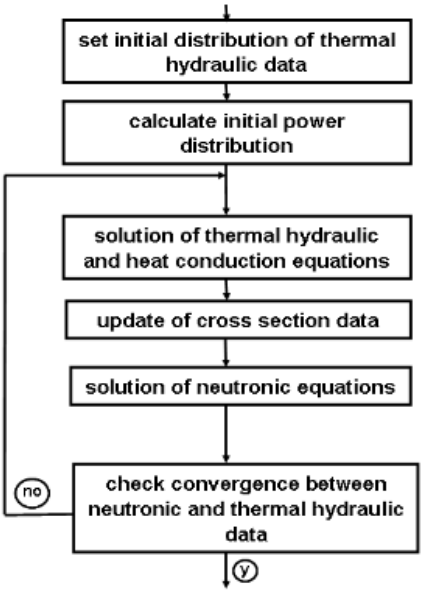
### CRONOS2/FLICA4 [73]:

In CRONOS2/FLICA4, the TH of the core can be dealt with in a simplified model inside CRONOS2 but it can also be treated more precisely by the FLICA4 code externally coupled with CRONOS2 through PVM. The synchronism of the codes is done at each time step through a semi-implicit time scheme for the coupling with variable time steps.

### DYN3D-SP3 (coupled) [46] [9]:

Even though DYN3D is a code devoted to core analysis, it has been placed in coupled codes since it has a TH module. For steady state an iterative solution approach is selected. DYN3D calculates the initial power distribution based on a set of initial TH data. FLOCAL is called to solve the TH and heat conduction, which is a critical step for updating the cross section data. Once this is done the N equations are solved to obtain the new power distribution which will be used by FLOCAL to update the TH parameters. This iterative process is shown in Figure 8.

Figure 8: Standard iteration scheme in DYN3D for steady state calculations. [46]

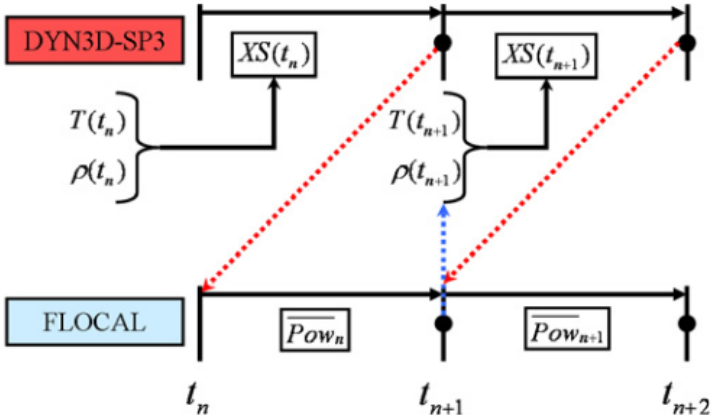



For the temporal analysis, an operator splitting approach has been followed. The new power distribution is first calculated by means of the N solver. In the case of FLOCAL, the power densities at the beginning and end of the TH steps are needed as an input, however, the average value of the two power densities are used as shown in equation 46.

$$\overline{Pow_n} = \frac{Pow_{t_n} + Pow_{t_{n+1}}}{2}. \tag{46}$$

A simplified view of the coupling in DYN3D standalone, with the FLOCAL TH model is presented in Figure 9 [11].

Figure 9: Steady state coupling of DYN3D-SP3 with FLOCAL [17].

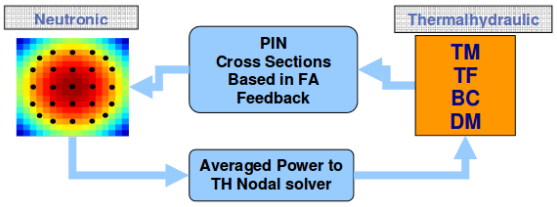



However, for a detailed transport solution at pin level with DYN3D-SP3, pin based cross sections are needed. If the solution is a time dependent one, then the cross sections must be generated in advance for the expected range of TH parameters such as fuel temperature, coolant density, boron concentration,

[11] Definition of the parameters used are presented in DYNSUB, previously mentioned in this section. Also refer to figure 11.

etc. The one dimensional TH module, FLOCAL, is able to predict these feedback parameters at a nodal level i.e. averaged over one fuel assembly. As can be seen in figure 10, the neutronic solution is a detailed one while the TH solution calculates nodal averaged values at the fuel assembly level. By this approach detailed information is lost. In this figure the parameters TM, TF, BC and DM are the moderator temperature, fuel temperature, boron concentration and moderator density respectively.

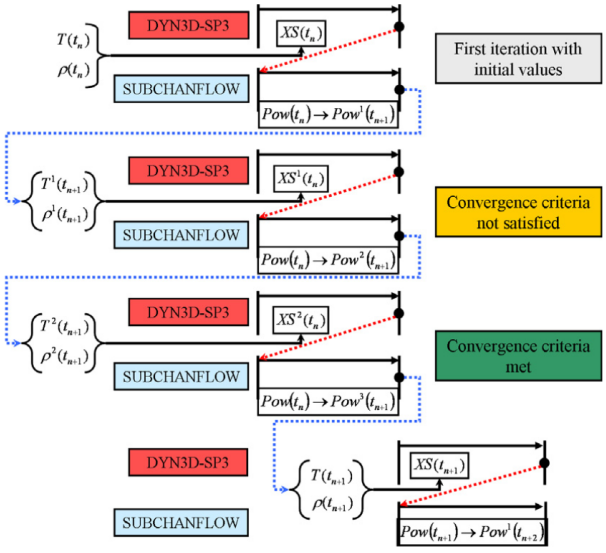
Figure 10: Time dependent coupling of DYN3D-SP3 with FLOCAL [17].




**DYNSUB** [17]:

DYNSUB is a novel two-way pin-based coupling of the simplified transport (SP3) version of DYN3D with the sub-channel code SUBCHANFLOW. The new coupled code system allows for a more realistic description of the core behavior under steady state and transients conditions. Additionally to the explicit coupling developed, a nested loop iteration or fixed point iteration (FPI) is implemented in DYNSUB. A FPI is not an implicit scheme but approximates it by adding an iteration loop to the current explicit scheme. The advantage of the method is that it allows the use of larger time steps (optimization of computational times without losing accuracy); however the nested loop iteration could take much more time in getting a converged solution and could be less efficient than the explicit scheme with small time steps. It is also shown that a FPI scheme can produce inaccurate results if the time step is not chosen in agreement with the analyzed transient. In the following figure $XS^n(t_n)$ represents the cross sections obtained by the $T(t_n)$ and $\rho(t_n)$ parameters (temperature and density at time $t_n$ respectively). DYN3D calculates the core power $Pow(t_n)$ and SUBCHANFLOW calculates the new TH conditions from this parameter. Convergence is checked at each time iteration step based on the total power, and TH parameters such as Doppler temperature and coolant density.

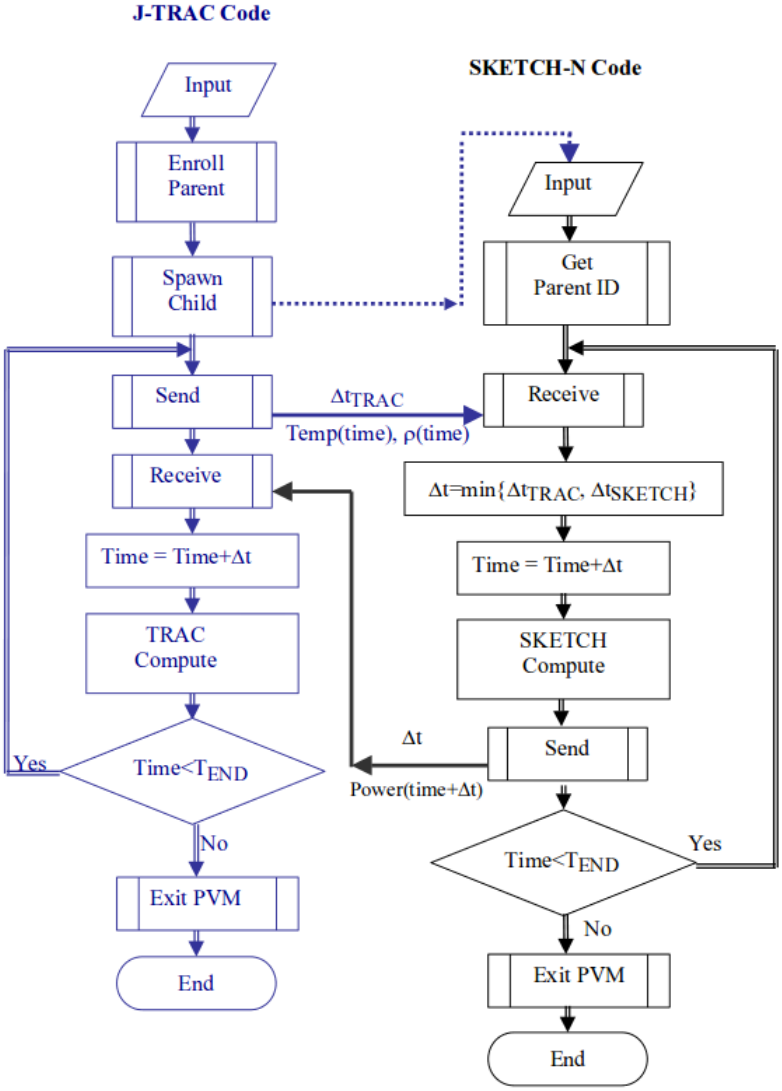
Figure 11: DYNSUB: FPI coupling scheme between DYN3D and SUBCHANFLOW [74].



**J-TRAC/TRAC-BF1/SKETCH-N** [75]:

In J-TRAC/TRAC-BF1/SKETCH-N the marching scheme based on an external coupling and data transfer between the codes is organized using the message passing library PVM. The codes are treated as separated processes and the subroutines based on PVM are responsible for a data exchange between the codes and a synchronization of time stepping. After performing an input, the J-TRAC code enrolls into PVM and spawns the child process – SKETCH-N. When SKETCH-N starts, it gets an ID number of the parent process and the code can communicate to each other sending/receiving messages. At the beginning of a time step, J-TRAC sends a message to SKETCH-N with TH reactor data and an estimation of the next time step size. SKETCH-N receives the message, selects a new time step size and performs the neutronic calculation. In TRAC-BF1/SKETCH-INS, the code is assembled by coupling both, which is also based on the message-passing library PVM. The interface module is responsible for data transfer between the codes, mapping of the data between different spatial meshes and synchronization of the time stepping.

Figure 12: Flow chart of the J-TRAC/SKETCH-N calculation [62].



**MOOSE** [76] [4]:

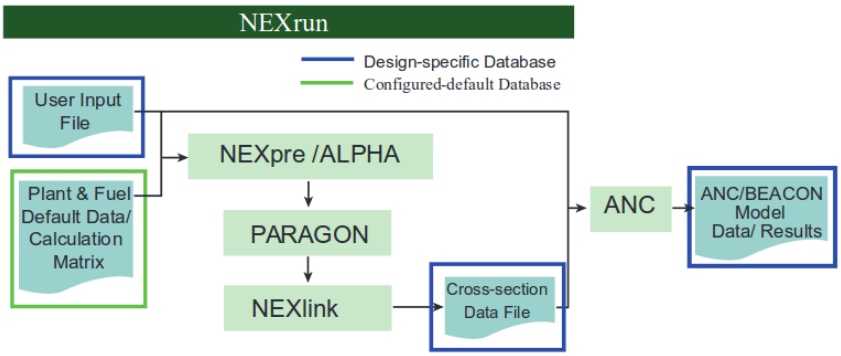
The Multi-physics Object Oriented Simulation Environment (MOOSE) is based on solving all systems in a fully coupled manner using the JFNK method with pre-conditioners. The design of MOOSE capitalizes on the fact that the unpreconditioned JFNK implementation requires only residual evaluations of the discretized system. Utilizing the mathematical structure present in JFNK, physics are modularized into "Kernels" (each in charge of a task). Each Kernel can also optionally provide a Jacobian or preconditioning matrix which can then be used for physics based preconditioning of the matrix free calculation.

In addition, systems are solved in a fully coupled and fully implicit manner employing physics based preconditioning which allows great flexibility even with large variance in time scales. For these reasons, MOOSE utilizes Krylov methods for solving the resultant linear systems. This allows for a modular architecture that greatly simplifies the addition of new physics and coupling them together. MOOSE includes an extremely flexible Physics Based Preconditioner (PBP) that can be utilized by any application built using MOOSE. The PBP allows for runtime configuration of all preconditioning options. Three main preconditioning schemes are usually employed by applications: operator split using only block diagonals, lower block triangular using one block Gauss-Seidel like iteration and variable block structure utilizing multiple block Gauss-Seidel iterations.

**NEXUS/ANC9** Code System [77] [78]: The next generation of Westinghouse core design systems.

It accurately and efficiently models and predicts core performance for all square-lattice PWRs, including the AP1000 PWR. The NEXUS code system is used to generate the cross sections which ANC9 needs for the neutronic simulation. NEXUS makes use of PARAGON, a 2D lattice physics code which allows the explicit modeling of current and future heterogeneous fuel designs. The code is able to deal with multi-region resonance self-shielding effect for all resonant isotopes in the fuel rods micro-regions including Gd spatial concentration variation due to burn-up depletion. Once the cross sections are prepared, ANC9, a multi-dimensional nodal code for nuclear core design, performs its calculation. For the TH, the ANC9 TH module calculates the enthalpy of each node based on the core node-wise power distribution, channel inlet temperature, and channel flow rate in an explicit approach. From the enthalpy of each node, ANC9 TH module obtains the moderator temperature and density distribution by directly looking up the steam table based on the local enthalpy and core pressure. However, an improved TH modeling by integrating the VIPRE-W TH code could be done. VIPRE-W is an enhanced version of VIPRE-01 (based on the COBRA family of codes). It solves the FD equations for mass, energy, axial, and lateral momentum for interconnected array of channels, assuming incompressible and thermally expandable homogeneous flow. Once again, the coupling is done following an operator splitting approach between VIPRE-W and ANC9.

Figure 13: Nexus code system iteration scheme [78].

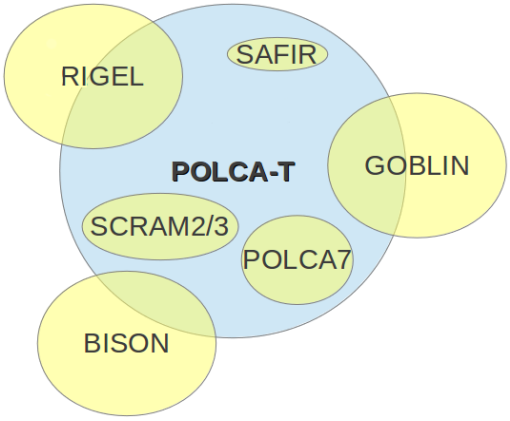



**POLCA-T** [12] (System Code):

The POLCA-T methodology is based on the combination of codes and methods. Generally speaking, it iteratively couples the POLCA7 N code with the RIGEL TH code. Moreover, the code utilizes models

of other Westinghouse BWR tools, such as fuel performance code, steam lines models and plant control models. It is suitable for applications concerning static 3D BWR safety analysis, core design, hydraulic loads, etc... and transient analysis, control rod drop accident, stability evaluation, ATWS, ATWC and LOCA analysis. It can also model cores containing MOX fuels. POLCA-T includes several models for reactor system components. These models include specific component models for turbo pumps, jet pumps, steam lines and steam separators. Figure 14 shows the general overview of the POLCA-T code.

Figure 14: General overview of the POLCA-T code [12].




A brief description of the codes that provide input to POLCA-T is presented hereafter:

1. RIGEL: Involves the code structure/code design and modeling approach of the TH.
2. SAFIR: Digital control simulation package.
3. SCRAM2/3: For simulation of the TH in the hydraulic SCRAM system, i.e. the control rod velocity prediction.
4. GOBLIN (BWR part): The Westinghouse LOCA code for BWRs applies the bases for the solution formulation and several models for the TH and heat transfer simulations.
5. POLCA7: The N that is used to calculate the fission power distribution of the core.
6. BISON (BWR part): Provides the methodology to calculate CPR in BWR cores.

Furthermore, some specific applications have been simulated and involve;

- special studies for stability performance: Innovative fuel design, fuel bid.
- 3D transient methodology studies.
- Nuclear heating events in BWRs: generic studies, specific plant events.
- Simulation of ATWS and ATWC in the Nordic countries.

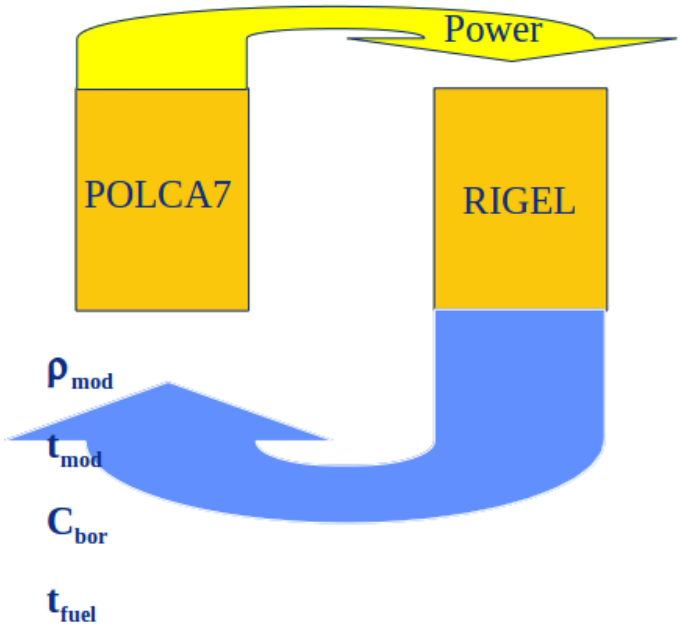
POLCA-T uses an object oriented topological input deck, and the code is fully programmed in FORTRAN 95/2004. It provides a consistent formulation for the steady sate and transient calculations, meaning, the use of the same equation sets. For determining the Doppler reactivity, POLCA-T uses the volume average nodal fuel temperature. The basic solution technique for POLCA-T is based on a state variable vector concept that tracks the TH nodal parameters. These parameters are coupled with the hydrodynamic field equations and neutronic models to determine rates of change in the vector quantities for a series of volume cells. The flow paths are described by the cross vapor and liquid velocities. The steady state and transient calculations are performed in a similar manner. The steady state solution technique is a special case of the transient solution where the time derivative terms of the functions, mass, energy, etc... are set to zero. The code linearizes the time domain response for each state variable. The field equations, closure relationships, and associated models provide the basis for determining the rates of change in variable quantities. POLCA-T includes options for both implicit (1st order as default, however a more

accurate 2nd order degree could be used) and semi-implicit time integration methods for calculating the transient response. The time step limit and control is established based on Courant limit checks, material properties out of the desired range and on state variable derivatives. When an automated time step control option is used, the time step decreases if the accuracy within successive iterations is outside a user defined allowable value. Furthermore, accuracy is ensured by controlling time step and number of iterations though convergence criteria. There is a separated default convergence criterion in POLCA-T based on a rod surface temperature difference.

The mass and energy equations for the phases, momentum equation, and drift flux correlation for each flow path along with the pump speed equations are solved simultaneously using Newton's method. The Jacobian matrix includes all derivatives and is inverted using a sparse matrix technique. The heat structure conduction equations are solved by Gaussian elimination and back substitution. The conduction equation and the surface heat transfer are solved iteratively for the surface temperature. The 3D kinetics model is solved using an iterative method and is then iterated in an outer loop including the TH equations until convergence is reached. The hydraulic model can be solved using a fully implicit or semi-implicit method. The thermal conduction and heat transfer models are solved using a method that is implicit in time. The hydraulic fluid conditions are treated implicitly in the heat conduction and heat transfer solution. The surface heat transfer, however, is treated explicitly in the hydraulic solution.

The code is an internal coupled scheme of N and TH modules. The coupling is based on the use of the very same TH equations for core and plant system models through arrays that store data structure for communication between the two codes. Proper drift flux correlation are specified for each model, and if required for any of its fluid nodes. The code also integrates a multi-scale geometrical flexibility. On the micro level there are models in the core: fuel, gas gap, and cladding, fuel assemblies, pin power, core bypass, etc. At the macro level, it covers the RPV, recirculation loops, MSL, steam bypass lines and other plant models. This geometrical flexibility allows the code's application to a wide range of plant designs as well as to separate test facilities. For the temporal coupling, one TH time step per each neutronics step, i.e. at each time both TH and neutronics solutions are obtained, is used. A semi-implicit second order numerics scheme is implemented. Finally, each hydraulic channel that models the fuel assembly has one heat structure for the fuel rod, one for the water channels (if any are presented) and one for assembly box. A one to one mapping for both in radial and axial planes is implemented. Figure 15 shows the coupling approach followed by POLCA-T.

Figure 15: POLCA-T computational procedure.

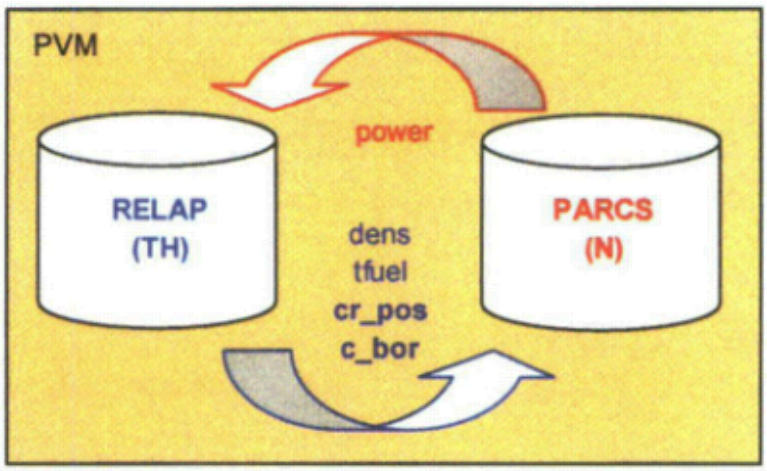


**RELAP5** - coupled with the N codes:
DYN3D [63] - PARCS [79],[80] - KAPROS [81] - PANTHER [82] -PANBOX [83] [84]:

In RELAP5/DYN3D the communication is preserved by external coupling between both codes. RELAP5 models the whole NPP without core kinetics. Selected TH data are transferred from the RELAP part of the coupled code to DYN3D. These are core inlet temperature, inlet mass flow rate, boric acid concentration as well as core outlet pressure and core pressure drop. The main results of the core calculation, specially the linear power rate, are transferred to the thermal structures (TH part of the coupled code). Additionally, reactivity and total power are transferred. The exchanged data are updated periodically. The time data (time step, actual time and total time of calculation) are controlled by the TH part (RELAP5) that acts as time manager controlling the main time step and the total time of calculation. Information about actual time and time step is transferred to the core N model.

The coupled RELAP5/PARCS code utilizes an internal integration scheme in which the solution of the system and core TH is obtained by RELAP5 and only the spatial kinetics solution is obtained by PARCS. In this scheme, PARCS utilizes the TH solution data (e.g. moderator temperatures/densities and fuel temperatures) calculated by RELAP5 to incorporate appropriate feedback effects into the cross-sections. Similarly, RELAP5 takes the space-dependent powers calculated in PARCS and solves for the heat conduction in the core. The temporal coupling of RELAP5 and PARCS is explicit in nature, and the two codes are locked into the same time step. For this implementation, the RELAP5 solution lags the PARCS solution by one time step. Specifically, the advancement of the time step begins with RELAP5 obtaining the solution to the hydrodynamic field equations using the power from the previous time step. The property data obtained from this solution is then sent to PARCS and the power at the current time step is computed. The coupling between PARCS and the TH code is achieved by the interprocess communication protocol, Parallel Virtual Machine (PVM). The two processes are loaded in parallel and the PARCS process transfers the nodal power data to the TH process. The TH process then sends back the temperature (fuel and coolant) and density data back to the PARCS process. Originally, it was necessary to execute a third intermediate process, which manages the data transfer between the two processes. But this process has been integrated into PARCS so that only two processes are to be run in parallel. For RELAP5/PARCS, the coupling is based on an internal scheme, at which the TH, heat conduction and N interact. In fact, for this case the heat conduction equations are solved first. Then the results are passed to the TH and N equations. Explicit coupling numerics for steady state and transient are used. The maximal time step size is 0.01 s and the convergence criteria is 0.001 for steady state solutions on TH parameters. In the following figure, "dens" is the coolant density, "tfuel" represents the fuel temperature, "cr_pow" the control rod position and "c_bor" the boron concentration.

Figure 16: Parallel execution scheme between RELAP and PARCS [85].




In RELAP5/KAPROS, the super-cell model from KAPROS is coupled with the TH system code RELAP5, being improved for Hight Performance Light Water Reactor (HPLWR) applications. The RELAP5 input model describes the whole reactor system, including a one-channel representation for the core. In this

case the fuel assembly model for the neutron physics calculations seems to be adequate. The coupled calculations start with a cosine shape estimate for the power distribution along the axial length in the RELAP5 core model. The resulting axial distributions of the densities of the fuel and coolant and of the temperatures of the fuel, the clad and the coolant in these zones of the model are extracted from the RELAP5 output and processed to input for the KAPROS cross section generation. These cross sections are used for the calculation of an axial power distribution in the super-cell fuel assembly model with the TWODANT[12] code. The feedback of this new axial power distribution to the RELAP5 calculation may be repeated as many times as desired by input. The coupling of these codes RELAP5 and TWODANT is organized within the KAPROS system.

For RELAP5/PANTHER, the coupling is a simple extrapolation of existing technologies permitted by the fact that the codes are executed as separate processes and that they only interact throughout their respective boundary conditions (explicit in nature). This particular feature ensures that the numerical properties of the solution algorithms implemented in each code are entirely preserved by the coupling mechanisms. In particular, each code preserves its own time integration scheme: a leapfrog feedback technique used in PANTHER and the semi-implicit scheme in RELAP5. The data transfer technique between PANTHER and RELAP5 can be approached using two methods.

In the first one, each code uses at the beginning of the time step the boundary conditions computed at the end of the previous time step by the other code. Considering the respective time advancement for PANTHER and RELAP5, the data transfer is considered as a simultaneous process. In the second method, the TH transfer is one time step ahead of the neutron kinetics. This allows PANTHER to use implicitly boundary conditions evaluated by RELAP5 at the end of the time step, while RELAP5 uses boundary conditions at the beginning of the time step. Considering the respective time advancement for PANTHER and RELAP5, this data transfer can be considered as a TH lead process. For TH driven transients/accidents like SLB or feed water-line break, however, both schemes provide identical solutions at numerical convergence in the data transfer. Because of the external coupling, the domain of application of the coupled package is ensured by the common domain of each code. RELAP5 is validated for a wide range of plant transients and accidents including MSLB.

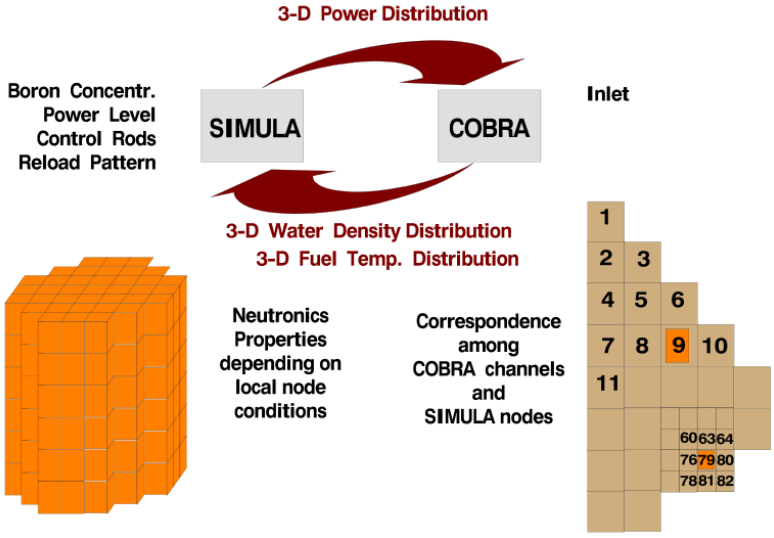
The PANTHER core TH is designed to cover applications where void effects are not dominant, which is the case of the non-LOCA licensing applications. The only caution required by the user is to build a nuclear data library structure that covers the whole range of coolant densities of the simulated transient. In RELAP5, the time step definition is subject to the material Courant limit or stability constraints, and the maximum calculation time step usually varies. Such limitation also exists in the implicit scheme of the PANTHER 3-D kinetics solution technique linked to a semi-explicit scheme for core TH. Consequently, the time step is usually larger in PANTHER than in RELAP5, in spite of the smaller time constants in the neutronics than in the TH. Because core boundary condition updates are needed at each PANTHER time step, the RELAP5 minor edit frequency is synchronized on the PANTHER time discretization. The latter must be chosen to ensure the best trade-off between computation time and accuracy. In practical applications, PANTHER and RELAP5 are installed on separate workstations, and all the data are exchanged by files across the local area network. If this coupling technique generates a significant increase in execution time for each run due to file exchanges, it however simplifies code installation since each code is used in its usual stand-alone application configuration and environment. For RELAP5/PANBOX (a nuclear plant safety analysis code system) both codes follow an explicit feedback scheme.

[12]TWODANT is a 2D neutron transport code developed at Los Alamos National Laboratory.

**SIMTRAN** [86]:

In SIMTRAN, the code merges the 3D neutronic nodal code SIMULA and the multi-channel with cross flows TH code COBRA-III. Both codes solve the 3D neutronic and TH fields with maximum implicitness using direct and iterative methods for the inversion of the linearized system. The coupling is achieved internally through a semi-implicit scheme which uses a staggered alternate time mesh.

Figure 17: SIMTRAN: Coupling scheme between SIMULA and COBRA-III [86].




**TRAC(-BF1/-PF1)** - coupled with the N codes:
COS3D [36] - ENTRÉE [87][47] / NEM [88]

The TRAC-BF1/COS3D is a best estimate coupled 3D core and TH code system. TRAC-BF1/COS3D is a coupled system of both codes, which are connected using a parallel computing tool. Instantaneous variables, namely, moderator density and fuel temperature are calculated at each channel component of TRAC-BF1. Those variables are transferred from TRAC-BF1 to COS3D via PVM. After COS3D calculates the neutronic condition according to those variables, it returns the power distribution data to TRAC-BF1, which then calculates TH condition in the plant based on the power distribution. Such a data transfer is executed by turns at every time step.

For TRAC-BF1/ENTRÉE, a parallel coupling system between the highly accurate 3D neutron kinetic code ENTRÉE and the versatile BWR simulator is achieved. A parallel processing between two codes will be realized by the PVM protocols that enable synchronization of data sending and receiving calls in two processes.

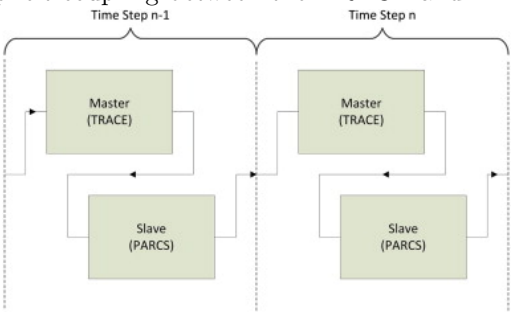
For TRAC-PF1/NEM, the TH code is the master time-step selector. It follows a semi-implicit method implying that the feedback parameters from an old time step and some from the new time step are used.

**TRACE/PARCS** [11]:

The TRACE/PARCS coupling includes a nested loop or FPI scheme. TRACE will be the master code and PARCS will follow and use the same time step. For fast steady-state initialization, a neutronic calculation skipping strategy is used, i.e. PARCS calculation is done only once per every 20 time advances in TRACE. SETS numeric scheme is used for steady-state calculations while explicit is used for the transient calculations. TRACE/PARCS coupling is performed using a general interface, which was implemented

using PVM. Overall controls of the coupled transient such as convergence checks and trip initiation are handled by TRACE.

Figure 18: Explicit coupling between the TRACE and PARCS codes [89].




**VIPRE-02/ARROTTA** [90]:

In VIPRE-02/ARROTTA, the code is used for the 3-D kinetic analysis of transients where only the core dynamical behavior is of interest. The reason is that the code is principally built on an explicit coupling between the ARROTTA 3-D neutronic code with the VIPRE-02 TH code and aimed at performing steady-state and transient analyses of full core models.

# 4 Conclusions

Due to the strong coupling between the neutrons and thermal-hydraulics system of equations (and physics), a need to better understand this coupling is a fact. The type of interaction between codes (feedback exchange and time advancement) is an critical issue to consider while doing coupled calculations in order to obtain accurate results within reasonable computational time. A very consistent literature review was presented in this report. The following table summarizes the stand alone codes encountered, their application area and numerical approach to solve their system of equations and/or discretization technique.

Table 2: Summary of the reviewed numerical schemes.

| Physics | Numerics | Spatial(order) | Temporal(order) |
|---|---|---|---|
| Fluid flow | FD/FV | 1 | 1 |
| Heat transfer | FD | 2 | 1 |
| Neutron diffusion | specific | - | 2 |
| Precursor concentration | FD-Crank-Nicholson | - | 2 |

The report provides a clear understanding of current coupled systems and their coupling principle. From this survey (stand alone or coupled codes), a summary of the most generally used numerics aiming to solve the different physics and domains is presented in the following table.

On the coupling side, internal and operator splitting coupling approaches are the most mature techniques implemented. New numerical algorithms refer to the fully implicit JFNK method, currently implemented in MOOSE, which provides a new type of solution in order to avoid errors cause by non-linearities and memory saving. Finally, the reader should be aware of the fact that another report titled "Survey of the state of the art numerical techniques for solving coupled non-linear multi-physics equations" exists and more details about coupling techniques are presented there.

Table 3: Summary of the revised codes.

| Code(s) | Physics | Numerics |
|---|---|---|
| ATHLET | TH | FEBE |
| ARROTTA | N | ANM/BiCGSTAB |
| BIPR8NK | N | NEM |
| CATHARE | TH | FV/implicit/ICE |
| COBAYA3 | N | FE/Crank-Nicholson/ACMFDM |
| COBRA-III | TH | FD/Newton Raphson - SOR |
| COS3D | N | NEM |
| CRONOS | N | FE/implicit |
| DYN3D | N | NEM/implicit |
| ENTRÉE | N | NEM/explicit |
| FLICA4 | TH | FV/implicit |
| FLOCAL | TH | FV |
| KIKO3D | N | Runge-Kutta/GMRES-BiCGSTAB |
| NEM | N | NEM/FD/explicit |
| NESTLE | N | NEM/FD/BiCGSTAB-LU |
| PANBOX | N | SANEM |
| PANTHER | N | NEM |
| POLCA-T | N-TH | ANM-FD |
| PARCS | N | CMFD |
| QUABOX/CUBBOX | N | Nodal Methods |
| RELAP5 | TH | FD/semi-implicit |
| SIMULA-3 | N | SANM/implicit |
| SIMULATE-3k | N | FD |
| SKETCH-N | N | SANM/implicit/SOR |
| SUBCHANFLOW | TH | FV/SOR |
| TRACE | TH | FV/semi-implicit/SETS |
| TRAC-BF1/PF1 | TH | FD |
| VIPRE-02 | TH | Fully implicit |

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