FD: Finite Difference Toolkit

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1 Introduction

FD is a set of Maple [1, 2] routines and definitions designed to handle various tasks in applying finite difference techniques in solving partial differential equations (PDEs). Particularly, it is developed to provide a methodology and a syntactic language to solve time dependent or boundary value PDEs arising in physics. Solving a PDE involves various complications, including finding the correct finite difference approximation (FDA) to a specific accuracy, dealing with boundary points on the discretized numerical domain, initialization, developing testing facilities for insuring accuracy, and finally creating routines to solve the FDA equations over the numerical domain. FD is designed to simplify these steps while providing full control over the entire process, allowing the user to focus on the underlying physical phenomena. Specifically, FD is not created to be a "blackbox" PDE solver, rather it provides a mixed level of automation and user controlled definitions.

FD is still under development and was originally designed to be used in the numerical relativity research where the computational task to numerically solve the Einstein's equations [1], is rather challening. Keeping that in mind, FD was developed to deal with PDEs and differential expressions that are lengthy (in some case thousands or tens of thousands of expressions) and are usually machine generated to avoid human error. Therefore, FD is written in the Maple language, which provides a powerful symbolic manipulation envirounment and unifies the process of deriving the continuum form of the PDEs, and applying finite difference methods to create a discretized form. Furthermore, FD is built to directly parse a given differential expression[2] in its canonical continuous form [3] in Maple. This eliminates the need for having another high-level specification to define a PDE which can be a cumbersome task for the user, especially if the PDEs are derived from tensorial equations – such as PDEs arising in general relativity. This prevents potential human errors in transfering the equations from the symbolic calculation enviroument to the target "PDE solver" envirounment. In addition, FD inherits all of the capabilities of Maple language to deal with PDEs and algebraic expressions. In particular, the user can manage their working enviroument using Maple's built-in data and control structures and use *PDEtools* package to implement various other tasks such as coordinate transformation and checking for the consistency of the equations.[4]

After posing a PDE as a set of FDA equations over a discretized domain, these equations can be solved using FD's default *point-wise Newton-Gauss-Sidel* relaxation algorithm (see Sec. 2.2) – which is a common method in solving nonlinear time dependent PDEs. FD generates Fortran subroutines (and C wrappers) to perform the relaxation and may be used as a rapid prototyping tool to implement various finite difference schemes to solve a PDE. It also provides a rapid development workflow to create routines to evaluate the residual of the given FDA expression as a diagnostic tool.

FD is capable of dealing with the boundaries of the numerical domain by providing a syntax to specifiy the PDE or boundary conditions differently at different parts of the discetized domain. This allows the user to impose various boundary conditions such periodic boundary conditions, asymptotic behaviour boundary conditions or inner boundary conditions. This, particularly, is achieved in FD by implementing an equivalent method to the ghost cell technique used in finite difference methods, and

[1] A set of 10 highly complex and non-linear coupled PDEs that govern the dynamices of the curved spacetime in strongly gravitation objects like blackholes or neutrino stars.

[2] PDE, written in the from: $D(f) = 0$, where D is a differential operator and f is the unknown function, would be a special case of a differential expression that is equal to zero.

[3] An expression in which derivatives are presented using Maple's `diff` operator. An example of such expression is: `diff(f(t,x),t,t) - diff(f(t,x),x,x)`

[4] We note that GRTensor [3] Maple package is avaiable for dealing with tensorial partial differential equations and tensor manipulation.

can be used to create inner boundary conditions that arise from the symmetries in the system – such as requesting particular functions to be even or odd in specific coordinate direction.

In FD's envirounment, specifying the finite difference scheme by the user is as simple as merely providing the order of accuracy and limitation on the allowed grid points in the Finite Difference Molecule (FDM). FD has a simple internal algorithm to determine the number of points required to do "forward", "backward" and "centered" finite differencing of a given partial differential expression with the given accuracy. It ensures that the generated stencil expression has accuracy that is equal to the user specified value or better. The computed stencils are all stored in an internal table and are user accessible to be monitored for their order of accuracy and form.

Finally, FD produces Fortran routines (and C wrappers) that are parallel-ready and can be used in the framework of a high performance computing infrastructure. This is achieved by passing boundary flags to the routines which specify if the boundaries of the grid are between CPUs or are real physical boundaries. FD adopts PAMR's [4] standard in this matter, but any other parallelization framework should also have a similar method to deal with the inner CPU boundaries. We note that the Fortran routines generated by FD use only the basic data types of Fortran language and creating wrappers to communicate with them from a different language should be a straightforward task. By default, FD generates the C language wrappers which is one of the most common languages in high performance computing.

This user manual describes all of the features mentioned above and introduces the syntax of FD for posing a PDE as a finite difference equation with the given boundary conditions. First, two algebraic types are defined which are the fundamental objects that FD uses to identify a finite difference expression. These types are the building blocks that FD uses to directly translate a PDE to a discretized equation and eventually to Fortran routines. Then, a derived Maple table is introduced that specifies the PDE and the boundary conditions over the discretized numerical domain. Finally, we present the utilities FD provides to choose a finite difference scheme, compute the FDA equivalent of a given PDE and create Fortran codes to solve it. We assume that the reader has a working knowledge of Maple programming and is familiar with the basic concepts of finite difference methods. Some of these concepts are reviewed in Sec. 2. An experienced user may skip this section, while those who are not are encouraged to consult the references [1, 2, 5, 6].

2 Overview of Finite Difference Method

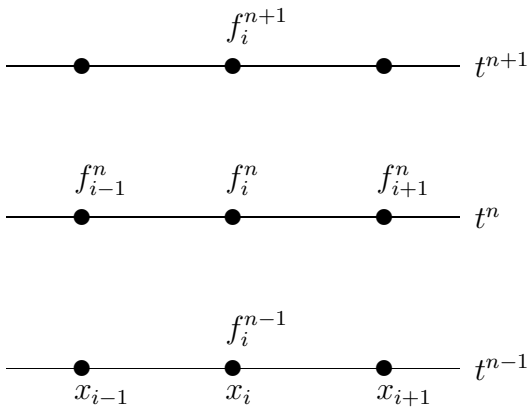
Finite difference methods are numerical techniques to express continuum differential expressions/equations as (approximate) algebraic expressions/equations. The resulting expression is known as the *Finite Difference Approximation* (FDA). An FDA for a derivative term, such as $df(x)/dx$, at a given point x, is a combination of the values of the function at certain points in the vicinity of x. For instance, values at the points $\{f(x), f(x+\Delta x), f(x+2\Delta x)\}$ (discretized values) can be used to approximate the first derivative of the function as:

$$\frac{df(x)}{dx} \approx \frac{-3f(x) + 4f(x+\Delta x) - f(x+2\Delta x)}{2\Delta x}\,, \tag{1}$$

where Δx is the *step size* of the discretization. This "scheme" is called *forward finite differencing*, as the discrete values are extended in positive(forward) x direction. Similarly, one can use the points $\{f(x), f(x-\Delta x), f(x+\Delta x)\}$ to compute the second derivative of the function,

$$\frac{d^2f(x)}{dx^2} \approx \frac{f(x-\Delta x) - 2f(x) + f(x+\Delta x)}{\Delta x^2}\,. \tag{2}$$

Here the point x is at the center, and thus the scheme is named *centered finite differencing*. The discretized points, $(\cdots, x-\Delta x, x, x+\Delta x, \cdots)$, construct a domain for an Ordinary Differential Equation (ODE) or a Partial Differential Equation (PDE). The following diagram illustrates this concept of *discretized numerical domain* for a 1+1 (1 spatial, 1 time) dimensional spacetime:



A discretization method transforms a function from a continuum form to a discrete form symbolized as:

$$f(t,x) \to f(t_n, x_i) \equiv f_i^n \,. \tag{3}$$

Here, we denote the time indexing with the superscript n and the spatial indexing using the subscript symbols (i,j,k). The grid structure, $\cup x_i \times \cup t^n$, (and similarly in higher dimensions add y_j and z_k) is usually considered to be uniform:

$$t^n = t^0 + n\Delta t \equiv t^0 + nh_t \,, \tag{4}$$

$$x_i = x_{min} + i\Delta x \equiv x_{min} + ih_x \,, \tag{5}$$

$$y_j = y_{\min} + j\Delta y \equiv y_{\min} + jh_y \,. \tag{6}$$

Using these symbols, a partial differential expression such as $\partial_x f(t,x)$ can be written as:

$$\frac{\partial f(t,x)}{\partial x} = \frac{f(t,x+h_x) - f(t,x-h_x)}{2h_x} + O(h_x^2) = \frac{f_{i+1}^n - f_{i-1}^n}{2h_x} + O(h_x^2) \,, \tag{7}$$

and the wording "approximation" is due to the neglection of the $O(h_x^2)$ term. Here the function $O(h_x^2)$ has explicit dependency of the from h_x^2 on the step size, and represents the error of the approximation (or equivalently can be interpretted as the "accuracy" of the FDA). Replacing all of the derivatives with FDA expressions, a PDE becomes an algebraic equation for the discrete values of the function. For example, consider performing the following FDA on the heat equation,

$$\frac{\partial f(t,x)}{\partial t} + \alpha \frac{\partial^2 f(t,x)}{\partial x^2} = 0 \quad \to \quad \frac{f_i^{n+1} - f_i^n}{h_t} + \alpha \frac{f_{i+1}^n - 2f_i^n + f_{i-1}^n}{h_x^2} = 0 \,, \tag{8}$$

where in the discretized version of the equation, the unknown is the vector:

$$\mathbf{F}^{n+1} = f_i^{n+1} \,, \tag{9}$$

and is to be solved numerically for a given $\mathbf{F}^n$. Obviously knowing the values $\mathbf{F}^1$, i.e the initial time profile of the function f, the process of solving $\mathbf{F}^{n+1}$ in terms of $\mathbf{F}^n$ means, by induction, finding the entire solution on the time domain indexed by n.

2.1 Computing the FDA Expression

There is a systematic method to find the FDA of the l'th derivative of a function, $d^l f(x)/dx^l$. Consider L points, in the vicinity of x as:

$$\{x + q_1\Delta x, x + q_2\Delta x, \cdots, x + q_L\Delta x\} \,, \tag{10}$$

where q_i's are L distinct integers usually chosen in a minimalistic fashion such that $x + q_i\Delta x$ is close to x. For example, the forward and centered finite differencing in Eq. (1) and Eq. (2) are associated with:

$$\{q_1, q_2, q_3\}_{forward} = \{0, 1, 2\} \;\;,\;\; \{q_1, q_2, q_3\}_{center} = \{-1, 0, 1\} \,. \tag{11}$$

Using these L points, and L unknown coefficients $\{\beta_1, \beta_2, \beta_3, \cdots, \beta_L\}$ one can create L Taylor expansions upto truncation error $O(\Delta x^L)$,

$$\beta_1 f(x+q_1\Delta x) = \beta_1 F^{(0)} + \beta_1 q_1 F^{(1)} + \beta_1 q_1^2 F^{(2)} + \cdots + \beta_1 q_1^l F^{(l)} + \cdots + \beta_1 q_1^{(L-1)} F^{(L-1)}\,, \tag{12}$$

$$\beta_2 f(x+q_2\Delta x) = \beta_2 F^{(0)} + \beta_2 q_2 F^{(1)} + \beta_2 q_2^2 F^{(2)} + \cdots + \beta_2 q_2^l F^{(l)} + \cdots + \beta_2 q_2^{(L-1)} F^{(L-1)}\,, \tag{13}$$

$$\vdots$$

$$\beta_L f(x+q_L\Delta x) = \beta_L F^{(0)} + \beta_L q_L F^{(1)} + \beta_L q_L^2 F^{(2)} + \cdots + \beta_L q_L^l F^{(l)} + \cdots + \beta_L q_L^{(L-1)} F^{(L-1)}\,, \tag{14}$$

where we defined:

$$F^{(r)} = \frac{d^r f(x)}{dx^r}\frac{(\Delta x)^r}{r!}\,, \tag{15}$$

and $F^{(0)} = f(x)$. Then we can find the coefficients $\{\beta_1, \beta_2, \beta_3, \cdots, \beta_L\}$ such that summing over the entire right hand sides of the equations, all of the $F^{(r)}$ terms have coefficients zero, except $F^{(l)}$ which can be set to have coefficient 1. This process leads to the following set of L linear equations for β_i's:

$$\begin{aligned}\sum_{m=1}^{L}\beta_m f(x+q_m\Delta x) &= F^{(0)}\sum_m \beta_m + F^{(1)}\sum_m q_m\beta_m + F^{(2)}\sum_m q_m^2\beta_m \\ &+ \cdots + F^{(l)}\sum_m q_m^l\beta_m + \cdots + F^{(L-1)}\sum_m q_m^{(L-1)}\beta_m = F^{(l)}\end{aligned}$$

$$\begin{aligned}&\Rightarrow\\ \sum_m \beta_m &= 0\\ \sum_m q_m^1\beta_m &= 0\\ \sum_m q_m^2\beta_m &= 0\\ &\vdots\\ \sum_m q_m^{l-1}\beta_m &= 0\\ \sum_m q_m^l\beta_m &= 1\\ \sum_m q_m^{l+1}\beta_m &= 0\\ &\vdots\\ \sum_m q_m^{(L-1)}\beta_m &= 0\end{aligned}$$

For L distinct given q_i's, this linear system has a unique solution vector which we denote by $\beta_i^\star$. Note that the left hand side of the summation is a finite difference expression:

$$\sum_{m=1}^{L}\beta_m^\star f(x+q_m\Delta x) = F^{(l)} = \frac{d^l f(x)}{dx^l}\frac{(\Delta x)^l}{l!} \Rightarrow \frac{d^l f(x)}{dx^l} = \frac{l!}{(\Delta x)^l}\sum_{m=1}^{L}\beta_m^\star f(x+q_m\Delta x)\,, \tag{16}$$

and therefore we find the desired FDA expression for the l'th derivative using L neighbouring points. In this calculation, clearly one should assume,

$$L \geq l+1\,, \tag{17}$$

which simply indicates that finding the FDA of a l'th derivative term requires at least $l+1$ points. The truncation error in the Taylor expansions is $O(\Delta x^L)$ and since the finite difference sum is divided by Δx^l in Eq. (16) the accuracy of the final finite difference expression is at least $O\left(\Delta x^{(L-l)}\right)$. However in certain cases (for example in centered scheme) the finite difference expression can have higher accuracy

as the coefficient in the next leading $O(\Delta x^L)$ term in the summation happens to simplify to zero. The reader may verify this for the FDA given in Eq. (2)

This calculation is internally performed by FD as it encounters derivative terms in a PDE and returns the FDA equivalent of them.[5] There is a simple front-end function (mostly for demonstration purposes) in FD:

```
Sten(diffexpr,[points])
```

which calls the internal FDA operator on the given differential expression, `diffexpr`, and computes the stencil using the points, `[points]`, (denoted by $\{q_i\}$ in the systematic derivation above). For example in the following we demonstrate the computation of the forward and centered FDA in Eq. (1) and Eq. (2) for the first and second derivatives respectively:

```
> Sten(diff(f(x),x),[0,1,2]);
                          -3 f(x) + 4 f(x + h) - f(x + 2 h)
                     1/2 ---------------------------------
                                       h
> Sten(diff(f(x),x,x),[-1,0,1,2,3]);
            11 f(x - h) - 20 f(x) + 4 f(x + 2 h) + 6 f(x + h) - f(x + 3 h)
       1/12 ------------------------------------------------------------------
                                          2
                                         h
```

Example 1: Simple FDA of derivatives using FD

We emphasize that this procedure is soley for demonstration purposes, and acts only on a single derivative term. In practice, FD uses a different procedure, `Gen_Sten`, that performs the FDA operation according to an FDA scheme specification provided by the user, and it performs on arbitrary length PDEs.

2.2 Iterative Schemes for Non-Linear PDEs

Solving a time dependent PDE for a function $f(t,\vec{x})$ involves integrating the equation forward in time, given the intial value $f(0,\vec{x})$. In the discrete language of finite differencing, this process reduces to finding the *advanced time level* value of the function, f^{n+1}_{ijk}, for the given *current value*, f^{n}_{ijk}. Starting with the "intial data", f^{0}_{ijk}, the time integration can be performed by applying this process consecutively for N_t time levels:

$$\text{Initial Data} \quad f^{n=0}_{i,j,k} \rightarrow f^{n=1}_{i,j,k} \rightarrow \quad \ldots \quad \rightarrow f^{n=N_t}_{i,j,k} \quad \text{Final State} \tag{18}$$

To demonstrate this update process, let's revisit the 1-D heat equation, with a different discretization scheme (known as leap-frog):

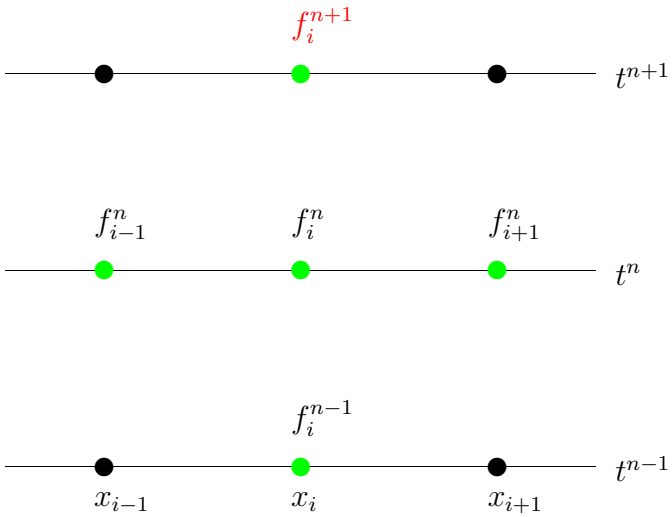
$$\frac{\partial f(t,x)}{\partial t} + \alpha \frac{\partial^2 f(t,x)}{\partial x^2} = 0 \quad \rightarrow \quad \frac{f_i^{n+1} - f_i^{n-1}}{2h_t} + \alpha \frac{f^n_{i+1} - 2f^n_i + f^n_{i-1}}{h_x^2} = 0\,. \tag{19}$$

This finite difference equation (FDE), is a second order approximation to the PDE at the point (t^n, x_i), and it involves values of the function at that point, and the points in the vicinity of it. The FDE includes the following points:

$$\{(n+1,i),(n-1,i),(n,i-1),(n,i),(n,i-1)\}\,. \tag{20}$$

and the"unknown" in this set, as highlighted in (19), is f_i^{n+1}. This set of points is called the *Finite Difference Molecule* (FDM) and is illustrated in the following diagram for the FDA of heat equation (19):

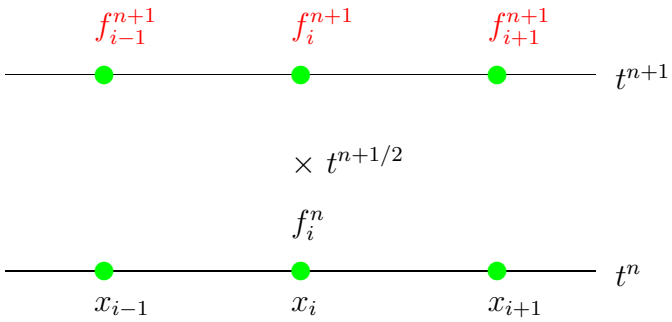
[5] We note that FD does *not* use any of Maple's substituition/replacement procedures, rather it performs recursively to parse a PDE and *return* FDA equivalents of its differential expressions.



FDM depends on the finite difference scheme. For example, consider a different (also second order accurate) FDA of the heat equation at the point $(t^{n+1/2}, x_i)$, where $t^{n+1/2}$ denotes the point $t_n + h_t/2$:

$$\frac{\partial f(t,x)}{\partial t} + \alpha \frac{\partial^2 f(t,x)}{\partial x^2} = 0 \quad \rightarrow \quad \frac{f_i^{n+1} - f_i^n}{h_t} + \frac{1}{2}\alpha \left(\frac{f_{i+1}^n - 2f_i^n + f_{i-1}^n}{h_x^2} + \frac{f_{i+1}^{n+1} - 2f_i^{n+1} + f_{i-1}^{n+1}}{h_x^2} \right) = 0\,. \tag{21}$$

The FDM of this equation is illustrated in the following diagram:



and again the unknown is highlighted both in the diagram and the equation. The main difference between this discretization and the previus one is in the fact that, this FDM requires 2 time level, whereas FDE (19) has 3 time levels. More importantly, in this scheme there are 3 unknowns in the FDA: $\{f_{i-1}^{n+1}, f_i^{n+1}, f_{i+1}^{n+1}\}$ and therefore there is an implicit dependency of advanced time level unknowns. This type of FD schemes are known as *implicit schemes*. The FD schemes such as the leap-frog scheme used in (19) – where the dependency of the FDM on the advanced time level is explicitly a single point – are known as *explicit schemes*.

After converting a PDE to a FDE, the next step is solving this algebraic equation. We can write an FDE in a compact form:

$$L_i^h \left(f_i^{n+1}, f_i^n, \cdots \right) \equiv \mathbf{L}^h \left(\mathbf{F}^{n+1}, \mathbf{F}^n, \cdots \right) = \vec{0}\,, \tag{22}$$

where $\mathbf{L}^h$ is the FDA operator, the most advanced time level values, f_i^{n+1}, is considered as the unknown, and the superscript h denotes the typical step size of the discretization. Here we defined the vector:

$$\mathbf{F}^{n+1} \equiv [f_i^{n+1}]\,. \tag{23}$$

Depending on the PDE and the chosen FDA scheme, this equation can be solved numerically using various methods. For a linear PDE and an explicit scheme, Eq. (22) is indeed a linear equation:

$$\mathbf{A}\mathbf{F}^{n+1} = \mathbf{b} \tag{24}$$

where $\mathbf{A}$ is a diagonal matrix and $\mathbf{b}$ is a vector that depends on previous time level values of the function, $\mathbf{F}^n, \mathbf{F}^{n-1}, \cdots$. In this case, solving the FDE simply reduces to inverting a diagonal matrix, i.e. inverting

the diagonal terms – which can be done in a single (trivial) matrix operation. But in general, if the PDE is linear and FD scheme is implicit, the FDE reduces to the same linear euqation as (24), but the matrix $\mathbf{A}$ is no longer diagonal. In even more general case, where the PDE is non-linear, and the FD scheme is implicit, one needs to solve a non-linear algebraic equation for a vector of unknowns. Such systems are perhpas the most interesting and are the subject of study with the FD toolkit.

In this scenario, one can solve the non-linear FDE using the multivariable iterative Netwon method:

$$\mathbf{F}_{l+1}^{n+1} = \mathbf{F}_{l}^{n+1} - \mathbf{J}^{-1}(\mathbf{R}_l) \tag{25}$$

in which the subsubscript l index's the number of Newton method iterations, i.e. $\mathbf{F}_{l+1}^{n+1}$ is the new approximate solution after a single iteration, and $\mathbf{F}_{l}^{n+1}$ is the old solution. In recursive Eq. (25), $\mathbf{J}^{-1}$ is the inverse of the Jacobian matrix of the FD operator $\mathbf{L}^h$ as a function of $\mathbf{F}^{n+1}$. More explicitly, it is the multivariable derivative of the nonlinear FDA operator $\mathbf{L}$:

$$\mathbf{J}_{ji} \equiv \frac{\partial L_j}{\partial f_i^{n+1}} \,. \tag{26}$$

Finally, in Eq. (25), ${}_l\mathbf{R}$ denotes the "residual" of the FDE for the previous approximate solution generated from the Newton iteration:

$$\mathbf{R}_l \equiv \mathbf{L}\left(\mathbf{F}_{l}^{n+1}\right) \,. \tag{27}$$

Note that this iterative method requires an intial guess that is usually taken to be the previous time step solution:

$$\mathbf{F}_{0}^{n+1} = \mathbf{F}^{n} \,. \tag{28}$$

Here the logic is simple: if the PDE evolves the function slowly in time, $\mathbf{F}^{n+1}$ is close to $\mathbf{F}^n$ and thus $\mathbf{F}^n$ should be a good initial guess for it. Note that in this method, each time level update demonstrated in (18) has another layer of Newton iteration presented in (25). This internal iteration usually converges very quickly (in few steps).

So far, we have only provided a formal description of solving a non-linear FDE. Practically, the numerical inversion of $\mathbf{J}$ is a non-trivial task. One can use the Gauss-Seidel or Jacobi methods to find the inverse matrix iteratively, however, since this Jacobian is going to be used in the Newton iteration (25) rather than performing two independet iterative schemes, one can simply find an approximate inverse Jacobian by only taking the diagonal part of this matrix and use that in the Newton solver. [6] This approach is called *point-wise Newton Gauss-Seidel* method and is equivalent to assuming that the only unknown in FDE is f_i^{n+1} (fixing the rest of advanced time level values that occur in an implicit FDA scheme) and solve for it using a single variable Newton method:

$$[f_i^{n+1}]_{l+1} = [f_i^{n+1}]_l - [R_{ii}]_l / J_{ii} \tag{29}$$

where:

$$[R_{ii}]_l = L_i\left([f_i^{n+1}]_l\right) \tag{30}$$

is the residual of the FDA equation at the point i and:

$$J_{ii} = \frac{\partial L_i\left(f_i^{n+1}, f_i^n, \cdots\right)}{\partial f_i^{n+1}} \tag{31}$$

is the diagonal element of the Jacobian matrix. Note that there are two iterations involved here, one over index i, the numerical grid, and one on the Newton iteration index l. It is ineffective to perform the l iteration first, since a highly accurate solution to the point-wise Newton problem will become completely disrupted as soon as the value of the next neighbouring point f_{i+1}^{n+1} is changed via the next Newton iteration. Therefore, it is much more effective to perform the iterating over the numerical grid first. This is known as a single point-wise Newton Gauss-Seidel *relaxation sweep* and if it converges, it usually only takes few iteration. Performing this relaxation, for few times, a single time step evolution is complete and the algorithm (18) can proceeed to the next step.

This algorithm is the first approach to solve a non-linear PDE and is the default (and at the moment only) method that is built into FD toolkit for solving the PDEs. As we will discuss in detail, invoking the procedure:

[6] The convergence of such method is guaranteed if the Jacobi matrix is diagnoally dominant, i.e. $\sum_{i=j} |A_{ij}| > \sum_{i\neq j} |A_{ij}|$

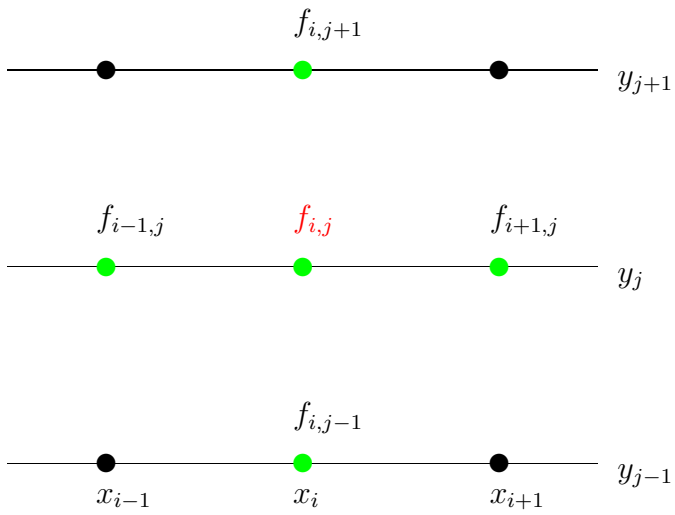
```
A_Gen_Solve_Code(DDS,{solve_for_var},input="d/c*",proc_name="my_proc")
```

will create a low level (Fortran) routine that performs the relaxation sweep. Having this routine, a PDE can be solved by a driver routine that applies the relaxation as needed (depending on some stopping criteria). Of course, solving a PDE involves several other steps, such as dealing with boundary points where rather than FDA equivalent of PDE, a boundary condition needs to be imposed. This is done by defining and passing the `DDS` variable which is a Maple data type to specify a PDE and its boundary conditions over a discreized domain. It is the description of the `DDS` and other tools and objects that are needed before applying this procedure that constitudes the majority of this documentation.

We note that a similar discussion to what we desribed about the time dependent PDEs also applies to the boundary value problem PDE's (elliptic PDEs). For example, consider the following second order discretization of the Laplace equation:

$$\frac{\partial^2 f(x,y)}{\partial x^2} + \frac{\partial^2 f(x,y)}{\partial y^2} = 0 \quad \rightarrow \quad \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{h_x^2} + \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{h_y^2} = 0\,. \tag{32}$$

The finite difference molecule for this FDA is illustrated in the following diagram:



In this case, one needs to provide the discrete values of the function at the boundary points, and the unknowns are all of the values in the interior points f_{ij}:

$$\text{(BVP)} \quad \{f_{1,j} \;\; f_{N_x,j} \;\; f_{i,1} \;\; f_{i,N_y}\} \;\rightarrow\; f_{i,j} \quad \text{(unknown)} \tag{33}$$

Again, a simple approach to solve this PDE is to use iterative schemes. For example, one can solve the FDA equation (32) for the mid-point value f_{ij}, assuming the values at the neighbouring points are fixed. Then performing this point-wise solver process over all of the interior points (a relaxation sweep) iteratively will decrease the residual to the desired tolerance (if it converges). However we note that relaxation schemes for boundary value problems (BVP) converge very slowly and other algorithms such as multigrid [4] are essential to efficiently solve elliptic-type PDEs.

2.3 Testing Facilities: Convergence and IRE

Finding a solution to a PDE or an ODE can be a complex task. However, if the solution is given as a discrete function, checking that it satifies the equation is somewhat a straightforward process. Consider the equation:

$$L(f) = 0\,, \tag{34}$$

where L is a differential operator and f is the unknown function. One can use an FDA scheme to discretize the differential operator:

$$L \rightarrow L^h \tag{35}$$

where h denotes the typical "size" of the discretization. Then for a given solution function, $\tilde{f}$, one can evaluate the residual:

$$R^h = L^h(\tilde{f}) \tag{36}$$

to confirm if the function $\tilde{f}$ satisfies the discretized version of the equation. A solid testing facility for a numerical solver is to *independently* develop this residual evaluator, which we refer as *Independent Residual Evaluator* (IRE). Of course, the residual (36) will not be exactly zero since L^h is an approximation to L and perhaps $\tilde{f}$ is also a numerical solution to (34) that differes from the exact solution f. However, one would expect if the solution $\tilde{f}$ is well resolved, is "close enough" to the exact solution, and FDA operator L^h is a "good" approximation of L, then the norm of this residual should be orders of magnitude smaller than the actual norm of the function $\tilde{f}$. A more rigorous definition of all these concepts and how to validate the numerical solution using an IRE test will follow. However, before that we momentarily dive into FD toolkit and how it provides a rapid workflow to creating IRE routines.

Consider the following ODE for $a(x)$ on a given time t:

$$\frac{da(x)}{dx} - \frac{1-a(x)^2}{2x} - \frac{1}{2}x\left[\left(\frac{\partial\phi(t,x)}{\partial x}\right)^2 + \left(\frac{\partial\phi(t,x)}{\partial t}\right)^2\right] = 0 \tag{37}$$

where $\phi(t,x)$ is a time dependent field which can have its own dynamical PDE. Here we want to evaluate the left hand side of the equation for the given discrete solutions a_i and ϕ_i^n and verify that it is zero (numerically). The process involves creating an FDA of this ODE, evaluating the residual over the numerical domain, summing up the point-wise residuals and returing a norm of it. FD toolkit provides an almost fully automated mechanism to do so. For example, if we use FD's default FDA scheme (second order accurate and centered), the Maple code to generate the IRE Fortran routine in this case is:

```
> read "FD.mpl": Make_FD():
> grid_functions:={a,phi}:
> res_a := diff(a(x),x)/a(x) - (1 - a(x)^2)/(2*x) -
     1/2*x*(diff(phi(t,x),x)^2+diff(phi(t,x),t)^2):
> Gen_Res_Code(res_a,input="c",proc_name="ire_a");
Fortran Code is written to ire_a.f
C header is written to ire_a.h
C call is written to ire_a_call
```

Example 2: Creating testing (IRE) routines with FD is fully automated.

The steps in this examples are: loading the FD package, initializing the internal variables of FD, defining symbols 'a' and 'phi' as grid functions, writing down the ODE, and passing the equation in its continuum form to the procedure:

```
Gen_Res_Code(expr,input="c*/d",proc_name="myproc");
```

This call creates 3 source code files:

- `ire_a.f`: is the Fortran subroutine that evaluates the residual (37). This subroutine has the following header:

  ```
  subroutine ire_a(a,n_phi,nm1_phi,np1_phi,x,Nx,ht,hx,res)
  ```

  and as you can see, it requires passing in the function a and 3 time levels of function ϕ, denoted by `n_phi` (current time), `nm1_phi` (retared time), and `np1_phi` (advanced time) since these values are required to compute the time derivative expression in the residual (in centered scheme). The last parameter `res` is a generic name, that always stores and returns the result of the computation (it will correspond to the updated value of the dynamical function when solver routines are generated).

- `ire_a.h` is the C header (wrapper) file that needs to be included in a C driver routine to use the subroutine, the content of this file is:

```
void ire_a_(double *a,double *n_phi,double *nm1_phi, double *np1_phi,
            double *x,int *Nx,double *ht,double *hx,double *res);
```

- `ire_a_call`: is a plain text file containing a typical C call of the routine. `_call` files can be copied to a C driver code. For example, here the content of the file is:

  ```
  ire_a_(a,n_phi,nm1_phi,np1_phi,x,&Nx,&ht,&hx,res);
  ```

  which as you can see, is a C call with the last parameter, again, labeled as `res`. After copying the content of `_call` to the driver code, the user needs to appropriatly change the name of the last parameter to the allocated vector (pointer) or the single variable defined in the C driver to store the result. [7] In this example, the result, `res`, is a number (a double precision floating point number) containing the norm of the residual. FD also assumes that in the C driver, the user will define the name of the allocated vectors and parameters for the PDE similar to what they are defined in the Maple expression.

We will discuss this procedure and similar other code generator procedures in more details through Sec. 3 to Sec. 6. Following note is a mathematical discussion on the notion of convergence and independent residual evaluators. Even though, these concepts are crucial to validate the consistency and accuracy of the numerical solver, the following is somewhat independent of the FD toolkit and applies to any finite difference method. This manual should be accessible without expertise in the mathematical discussion in the following note.

...

Note on convergence and IRE tests

Consider that the solution in Eq.(34) is produced by solving a finite difference approximation for the PDE. To preface this section, we first review our notation:

$$L(f) = 0 \tag{38}$$

$$S^h(f^h) = 0 \tag{39}$$

$$L^h(f^h) = R^h \tag{40}$$

i.e. L is the PDE operator in continuum form, and f is the continuum solution, f^h is the numerical solution and S^h is the solver FDA (the FDA of the original PDE that is used in the numerical solver). Finally, L^h is another FDA to L *that is different* than S^h, and due to this difference the RHS is nonzero and symbolized by the residual R^h. Note that previously we used L^h to denote the FDA used in the numerical solver, but here we are mostly interested in testing the solver using a different FDA operator which is the main focus of this section and thus denoted by L^h.

If the numerical solution f^h is convergent at the continuum limit – where the discretization size h approaches zero– we denote the continuum limit by u:

$$\exists u = \lim_{h\to 0} f^h \tag{41}$$

therefore one can assume the following Richardson expansion:

$$f^h = u + e_f^h = u + e_1 h + e_2 h^2 + \cdots \tag{42}$$

where the coefficients e_1, e_2 are functions independent of h. As one might expect, the error in the solution e_f^h depends on the accuracy of FDA S^h that is used in the numerical solver. The first non-zero coeffiecient e_p that appears in the expansion defines the accuracy of the solution, and is the dominent part of the error in the limit $h \to 0$. For example, a second order convergent solution has the form:

$$f^h = u + e_2 h^2 + \cdots \tag{43}$$

[7] Of course, a good strategy is to avoid naming any variables in the C driver code as `res`. The name `res` does not need any modification in the Fortran routine or C header file.

and using this expansion it is easy to show that for the 3 consecutively refined convergent solutions: f^h, $f^{h/2}$ and $f^{h/4}$ the limit of the following ratio:

$$\lim_{h\to 0} Q = \frac{||f^h - f^{h/2}||}{||f^{h/2} - f^{h/4}||} = 4\,, \tag{44}$$

is 4. Here $||.||$ is some norm of a discretized functions. Measuring the factor Q is refered as standard *convergence test* in the literature.

For a convergent numerical solution f^h, it is not clear that the limiting continuum function u (41) is indeed the solution to the continuum problem $L(f) = 0$, i.e. we want to know if:

$$u \stackrel{?}{=} f\,. \tag{45}$$

To further emphasize this: the numerical solution f^h might be convergent but we need some sort of proof to show that it is in fact converging to the correct solution. One might speculate that this should be the case if

1) S^h approximates L correctly, or more rigorously:

$$\lim_{h\to 0} S^h = L \tag{46}$$

known as *consistency condition* condition for the finite difference scheme.

2) The method used to solve the finite difference equation is *stable*. We refer the reader to [7] for mathematical definition and discussion on the notion of stability. In certain cases (for linear PDEs) it can be proven that stability and consistency are sufficient conditions for convergence. However, to our knowledege, there is no such proof for non-linear cases which most of the interesting physical systems exhibit. We also note that from a practical point of view there is no simple prescription or condition that can be checked off to ensure the stability of the method for non-linear systems.

Here we rather take a practical approach: the independent residual evaluation test. The IRE test provides a stronger test than the standard convergence test, and validates (or rejects) the equality 45. Suppose that f^h is $O(h^p)$ convergent, meaning:

$$\begin{aligned} f^h &= u + e_f^h \\ e_f^h &= e_p h^p + o(h^p) \end{aligned} \tag{47}$$

where e_p is a function, independent of h and $o(h^p)$ is an h dependent function that converges to zero faster than h^p:

$$\lim_{h\to 0} \frac{||o(h^p)||}{h^p} = 0 \tag{48}$$

Now suppose, as defined in the begining of this discussion in Eq. 40, L^h is another FDA of the original continuum operator L (created with a different FD scheme than S^h and is also created independently). L^h is what we refer as independent residual evaluator. We assume that this operator is *consistent* with the continuum operator L upto accuracy $O(h^q)$, meaning:

$$\begin{aligned} L^h(g) &= L(g) + e_L^h(g) \\ e_L^h(g) &= h^q E_L(g) + o_L(g; h^q) \end{aligned} \tag{49}$$

where E_L is an h independent operator, and $o_L(.; h^q)$ is an h dependent operator with a norm that converges to zero faster than h^q:

$$\lim_{h\to 0} \frac{||o_L(g, h^q)||}{h^q} = 0 \tag{50}$$

Note that here we are assuming that the operator expansion (49) is possible for the function g. Intuitively, one would expect this assumption to hold for functions that are well resolved over the discretized domain. Particularly in the case of $g = f^h$, this is a plausible assumtion, as we expect the numerical solver to produce a well-resolved discrete solution.

Now the claim is that if the conditions (47) and (49) hold then the residual defined as:

$$R^h \equiv L^h(f^h) \tag{51}$$

converges to zero if and only if f^h is indeed converging to f, the contiuum solution, i.e.:

$$u = f \tag{52}$$

Furthermore the convergence behaviour of the residual is dominated by the two errors: the solution f^h error, which we assumed to be $O(h^p)$ and the error of the L^h operator which we assumed to be $O(h^q)$ and is explicitly of the form:

$$||R^h|| = O(h^p) + O(h^q) = O(h^{min(p,q)}) \tag{53}$$

Therefore, for example if both the solution and the IRE are second order convergent then, one would expect to observe a second order convergence in the residual R^h as well.

Linear case:

We first proof the claim for the linear operators L and L^h which is rather simple:

$$\begin{aligned} L^h(f^h) = L^h(u + e_f^h) = L^h(u) + L^h(e_f^h) = L(u) + e_L^h(u) + L(e_f^h) + e_L^h(e_f^h) \\ = L(u) + h^q E_L(u) + h^p L(e_p) + h^q h^p E_L(e_q) + \cdots = L(u) + O(h^q) + O(h^p) + \cdots \end{aligned} \tag{54}$$

where $\cdots$ are higher order terms and we used the fact that L and L^h are linear operators, and from the definition (49) e_L^h is also linear. Note that in the expansion of the term $L^h(e_f^h)$, we are assuming that the error function e_f^h is also well resolved function on the mesh such that the expansion (49) is meaningful.

Nonlinear case:

In the nonliner case, a similar analysis can be performed by linearizing the FDA operator L^h. We assume that L^h is differentiable around g, meaning there exist a linear operator $\mathcal{D}_L^h[g]$ such that:

$$L^h(g + q) = L^h(g) + \mathcal{D}_L^h[g](q) + o_L^h[g](q) \tag{55}$$

and $o_L^h[g]$ is an operator with a norm converging to zero faster than $||q||$:

$$\lim_{||q|| \to 0} \frac{||o_L^h[g](q)||}{||q||} = 0 \tag{56}$$

The differential operator $\mathcal{D}_L^h[g]$ can be naively defined as the limit:

$$\mathcal{D}_L^h[g](q) \equiv \lim_{\epsilon \to 0} \frac{L^h(g + \epsilon q) - L^h(g)}{\epsilon} \tag{57}$$

Note that the differentiability of L^h is simply guaranteed if all of the partial derivatives $\partial L_i(g)/\partial g^{\tilde{i}}$ exist where L_i is the FDA equation at the point indexed by i and $g^{\tilde{i}}$ is the discrete value of the function at the point indexed by $\tilde{i}$. [8] These derivatives obviously exist for normal FDA operators used in finite difference methods. We also note that the abstract $\mathcal{D}_L^h[g]$ operator in a matrix representation is simply the $\partial L_i(g)/\partial g^j$ matrix. Furthermore, not surprisingly, it is equal to the FDA operator L^h itself, when L^h is linear:

$$\begin{aligned} \mathcal{D}_L^h[g](q) = \frac{L^h(g + \epsilon\, q) - L^h(g)}{\epsilon} = \frac{\epsilon L^h(q)}{\epsilon} = L^h(q) \\ \Rightarrow \mathcal{D}_L^h[g] = \mathcal{D}_L^h = L^h \end{aligned} \tag{58}$$

Note that in linear case, $\mathcal{D}_L^h$ indeed does not depend on g anymore, as the operator L^h. Assuming the differentiability of L^h around u, we have:

$$\begin{aligned} L^h(f^h) &= L^h(u + e_f^h) = L^h(u) + \mathcal{D}_L^h[u](e_f^h) + o_L^h[u](e_f^h) \\ &= L(u) + e_L^h(u) + \mathcal{D}_L^h[u](e_f^h) + o_L^h[u](e_f^h) \\ &= L(u) + h^q E_L(u) + o_L(u; h^q) + \mathcal{D}_L^h[u](e_p h^p + o(h^p)) + o_L^h[u](e_p h^p + o(h^p)) \\ &= L(u) + h^q E_L(u) + h^p \mathcal{D}_L^h[u](e_p) + o(h^p) + o(h^p) \end{aligned} \tag{59}$$

where in the last step we used the linearity of $\mathcal{D}_L^h[u]$ and the property of $o_L^h[u]$ operator (56). This result again translates to:

$$L^h(f^h) = L(u) + O(h^p) + O(h^q) = L(u) + O(h^{min(p,q)}) \tag{60}$$

[8] Note that here i and $\tilde{i}$ can be any of the discrete domain indecies, here we are simply using i as a symbol of discretization

and the residual $L^h(f^h)$ will converge to zero, if and only if $L(u) = 0$, or u the continuum function that the numerical solution f^h is converging to, is indeed the underlying continuum solution f.

Now using this result we have a stronger test: The convergence of the IRE $L^h(f^h)$ is only possible if the solution is convergent *and* is converging to the corret solution. Therefore if one can create a solid IRE operator L^h that is consistent with L, checking the convergence of the IRE will guarantee the accuracy of the solution. Of course, one can ask: what if L^h also has an error in its implementation ? Here the keyword *independent* development becomes crucial. If the independent residual is converging, it is exteremely unlikely that S^h and L^h that are developed completely independently both have an internal error, and both of the errors agree, i.e both S^h and L^h happen to be identical to an FDA for another PDE that is not the original PDE. Often it is best to create the IRE operator L^h using an automated process which is error-prone, this in part was the original motivation to develop FD and as it will be discussed further, generating IRE routines is been fully automated in FD toolkit.

3 Semantics of FD

In this section, we describe some of the internal variables of FD and two derived algebraic data types that FD uses to work with finite difference expressions.

3.1 Parsing a PDE: Fundamental Data Type

As mentioned in the introduction, FD is developed with the philosophy that user's involvement in the straighforward tasks should remain minimal. Consider the following PDE for f:

$$\partial_t f(t,x,z) + \beta(t,x,z)\partial_x f(t,x,z) + \gamma(x)\partial_z f(t,x,z) + a\partial_x^2 f(t,x,z) + b\partial_z^2 f(t,x,z) + g(x,z) = 0 \quad (61)$$

The LHS written in canonical Maple form (without use of aliases) is:

```
PDE:=diff(f(t,x,z),t) + beta(t,x,z)*diff(f(t,x,z),x)+gamma(x)*diff(f(t,x,z),z)
+ a*diff(f(t,x,z),x,x)+b*diff(f(t,x,z),z,z) + g(x,z);
```

One can easily observe that this expression, by itself, contains enough information regarding the dimentionality of the problem, functions and their dependencies, parameters, and of course derivatives. By looking at the expression, we can conclude that:

- f is a time dependent function, defined on a 2 dimenstional spatial domain labeled by (x, z).
- β is also time dependent with same spatial domain as f.
- g is a time independent function only defined on the (x, z) domain.
- γ has only 1 dimensional dependency on x coordinate.
- a and b are parameters (assuming that all dependencies are explicitly presented)
- the order and direction of derivatives of f are clear.

There is no need for further specification to pose this PDE to a computer, and the first step to reduce potential human errors is to eliminate another syntactic language to write a PDE. Rather, FD uses Maple's powerful symbolic manipulation capabilities and has a built-in parser which allows directly passing a PDE to its routines. This puts the entire complexity of the fundamental data type on the expression, and frees the user from providing any further specification. As soon as an error-proof PDE is written down, (which is easily possible as the working environment of FD is Maple with all its symbolic tools) the task of identifying the parameters, functions, dimensionalities, derivatives, and required time levels to perform FDA in time dimension is left to the software. This is one of the advantages of FD, over previously developed software such as RNPL [8]. This also makes FD an efficient prototyping language, particularly for developing testing facilities as we demonstrated in Example 2.

3.2 Coordinates

FD reserves the variables `(t,x,y,z)` for the name of the time and spatial coordinates that define the domain of a PDE. They are protected variables after FD is loaded. Similarly, FD reserves the symbols `(n,i,j,k)` for indexing the corresponding coordinate points `(t(n),x(i),y(j),z(k))`. It uses `(ht,hx,hy,hz)` as the name for the step-size of the discretization along these coordinates, respectively. The names `(Nt,Nx,Ny,Nz)` are reserved for the size of the discretized domain, and `(xmin,xmax)`, `(ymin,ymax)`, `(zmin,zmax)` are reserved for flags to specify the inner CPU boundary points of the coordinates (their applicable is in the context of parallelization).

This association can be demonestrated as:

$$\begin{aligned} t \leftrightarrow n \leftrightarrow h_t \leftrightarrow N_t \\ x \leftrightarrow i \leftrightarrow h_x \leftrightarrow N_x \leftrightarrow (xmin, xmax) \\ y \leftrightarrow j \leftrightarrow h_y \leftrightarrow N_y \leftrightarrow (ymin, ymax) \\ z \leftrightarrow k \leftrightarrow h_z \leftrightarrow N_z \leftrightarrow (zmin, zmax) \end{aligned} \tag{62}$$

and is built into FD. The coordinate names, and this association table are necessary to identify functions, differential expressions, and perform finite differencing. For example, FD recognizes that an expression such as `f(x+hx,y-2*hy)` should be discretized as `f(i+1,j-2)`, or an expression such as `f(x+hy)` is invalid and cannot be discretized, since `hy` is not an stepping size in `x` direction. Ultimately, this association table allows FD to discretize a differential expression such as $\partial_x f(x,y)$ (in Maple notation: `diff(f(x,y),x)`), directly to `(f(i+1,j)-f(i-1,j))/(2*hx)` without any need for further specification. (See the example in Sec. 3.4).

3.3 Initializing FD, `Make_FD, Clean_FD`

As the reader may have noticed from the previous examples, FD is in a Maple script format, and can be imported to a Maple worksheet/script by executing:

```
read("/your/fd/directory/FD.mpl");
```

FD's internal variables are initialized by calling the procedure:

```
Make_FD();
```

which has a short alias, `MFD()`, and creates the table for the coordinate association described in Eq. 62) and initializes the default finite difference table that specifies the finite difference scheme. We will further discuss this table in Sec 4.2. To clean the initialized variables, user can execute:

```
Clean_FD();
```

or use the alias `CFD()`.

3.4 Grid Functions Set: `grid_functions`

FD uses a global variable named `grid_functions` (of type `set` in Maple) as its reference for all of the function names that are expected to be discretized as:

$$f(t,x,y,z) \rightarrow f(t^n, x_i, y_j, z_k) \equiv f^n_{i,j,k}\,. \tag{63}$$

In Maple language, if symbol `f` is in the `grid_functions`, then the function `f(t,x,y,z)` (in its most generic 1+3 dimenstional case) will be converted to `f(n,i,j,k)` during the process of discretization. The following example demonstrates how FD uses the coordinate names, the coordinate association table, and the symbols defined in grid functions to produce FDA expressions:

```
> read "FD.mpl": MFD():
> grid_functions:={f}:
> Gen_Sten(f(t,x,y,z));
                                  f(n, i, j, k)
> Gen_Sten(diff(f(x,y),x));
                              f(i - 1, j) - f(i + 1, j)
                         -1/2 -------------------------
                                        hx
> Gen_Sten(x+g(y,z));
                              x(i) + g(y(j), z(k))
```

Example 3: Discretization of grid functions vs non-grid functions

Here, `Gen_Sten` is the main routine that performs the finite differencing and will be discussed extensively. However, user can easily guess its functionality from the example. As it can be seen, beside the names that are included in the grid function set, the coordinate variables `(t,x,y,z)` are by definition grid functions and are discretized as `(t(n),x(i),y(j),z(k))`. Furthermore, if a symbol with coordinate dependency (such as `g(y,z)` above) is *not* included in the `grid_functions` set, it will be considered as an external function that user will provide to the Fortran routines. FD discretizes its coordinate functions rather than the function. For example, here it is discretized as: `g(y(j),z(k))` rather than `g(j,k)`.

Time Level Reduction:
We shall emphasize that the discrete expression `f(n,i,j,k)` will be eventualy (at the point of code generation) replaced by: `n_f(i,j,k)`. This proceess is done internally, and is refered as *time level reduction* (See Sec. **??**). The time level `n` is usually refered as *current* time level, `n-1` is refered as *retarded* time level and `n+1` is called *advanced* time level. When FD performs the time level reducion, it uses the prefix `np1_` and `nm1_` in the names of the advance and retarded time levels functions respectively:

$$\begin{aligned} \texttt{f(n,i,j,k)} &\rightarrow \texttt{n\_f(i,j,k)} \\ \texttt{f(n+1,i,j,k)} &\rightarrow \texttt{np1\_f(i,j,k)} \\ \texttt{f(n-1,i,j,k)} &\rightarrow \texttt{nm1\_f(i,j,k)} \end{aligned}$$

The higher time level `f(n+2,i,...)` will be renamed to `np2_f(i,...)` and the syntax for the other cases should be clear. This replacement is simply because in time dependent finite difference algorithms only a finite number of time levels are needed and stored in the memory during the time evolution. The user can define the time levels in the C driver code according to this standard, or can define "alias" pointers (that adopts these names) to the underlying data structure to be able to use the FD generated routines.

3.5 Known Functions

FD has a set of "known" functions, which is basically a set of floating point functions that are known to the low level language (Fortran here). These functions in FD are:

```
{ln,log,exp,sin,cos,tan,cot,tanh,coth,sinh,cosh,exp,sqrt,‘^‘,‘*‘,‘+‘,‘-‘,‘/‘}
```

and during a discretization process, FD does *not* convert their arguments to a discrete version, rather it discretizes the arguments accordingly. For example, `sin(z)*f(x)+exp(y)` will be discretized as:

```
> Gen_Sten(sin(z)*f(x)+exp(y));
                              sin(z(k)) f(i) + exp(y(j))
```

assuming that `f` is in `grid_functions`.

3.6 Valid Continuous Expression, VCE

Valid Continuous Expression (VCE) is an algebraic function of the continuous coordinate variables, (t, x, y, z), in which the dependencies of grid functions on the coordinates are only of the form:

$$f(t + lh_t, x + mh_x, y + qh_y, z + ph_z)\,, \tag{64}$$

where (l, m, q, p) are known integers (not variable), and (h_t, h_x, h_y, h_z) are the associated stepsize variables. Furthermore, a VCE does *not* have explicit dependency on the discretiztion indices (n, i, j, k). For example, if functions `f` and `g` are grid functions, then all of the exressions:

```
f(t,x,y) + (g(x+hx)-g(x-hx))/(2*hx)
r(x*y)
u(sin(x*y),g(z))
f(x+2*hx,y-3*hy)/hz + x*z^2 + g(z,x,t,y)
```

are VCE, and

```
f(t,x+hy)
g(x,y+2)
f(x(i),y(j))
cos(j)
f(u(x),y)
g(x*y)
diff(f(x),x)
```

are all *invalid* continuous expressions. Particulary, compare `g(x*y)` and `r(x*y)`, former is not VCE, since `g` is defined as a grid function, while later is a VCE as r is considered an external function. Note that FD does not check for the consistency in the order of the variables, i. e. `f(x,y) + f(y,x)` is considered a VCE.

3.7 Valid Discrete Expression, VDE

Valid Discrete Expression (VDE) is an expression in which the explicit dependencies of functions on the discretization indecies `(n,i,j,k)` is only via the grid functions or coordinates. Furthermore, this dependency is of the form: $f(n+q, i+m, j+p, \dots)$, where $q, m, p, \cdots$ are known integers, and f is either a grid function or is one of the coordinates (t, x, y, z). In the case of coordinate, indexing must be done according to the coordinate-index association (62). For example, for `grid_functions:={f,g}`:

```
g(i+1,j-2)
x(i)
u(x(i),f(j,k),a)
f(j,k+2,i)
```

are all VDE and,

```
y(i)
x(i)+k
sin(i)
f(i*j)
u(i)
f(i,y(j))
```

are *invalid* discrete expression.

3.8 Conversion Between VDE and VCE

The definition of VDE and VCE allows a one-to-one mapping between these two types. FD provides two functions for the conversion:

```
A:=DtoC(B::VDE);
```

```
B:=CtoD(A::VCE);
```

Even though VCE's are not practically useful for numerical implementations, the conversion of a VDE to VCE can be used for demonstration and testing purposes. For example, a finite difference expression in VDE form, can be converted to a VCE, and then a taylor expansion of it can reveal its equivalent continuum differential operator. The following demonstrates the process for Kreiss-Oliger dissipation operator [7] that is commonly used in finite difference methods:

```
> read "FD.mpl": Make_FD():
> grid_functions:={f}:
> A:= -epsdis/(16*ht)*( 6*f(n,i) + f(n,i+2) + f(n,i-2)
                      -4*(f(n,i+1) + f(n,i-1))        ):
> B:=DtoC(A):
> E:=convert(series(B,hx),polynom);
                                                        4
                           epsdis D[2, 2, 2, 2](f)(t, x) hx
                 E := -1/16 ---------------------------------
                                       ht
```

Example 4: Conversion between VDE and VCE

which gives:

$$E = \frac{-\epsilon}{16}\left(\frac{\partial^4 f(t,x)}{\partial x^4}\right)\frac{h_x^4}{h_t} \tag{65}$$

4 Discretizing a PDE

In this section we discuss how to perform a finite differencing on a PDE using the facilities of FD, how to choose a specific discretization scheme and and how to access the results of a lengthy finite difference operation.

4.1 Performing the Finite Differencing, `Gen_Sten`

The main routine that performs FDA is:

```
VDE/VCE::Gen_Sten(expr)
```

(with an alias: `GS`) where the `expr` is an arbitrary mixed differential/algebraic Maple expression. As mentioned before, this routine performs the discretization on the grid functions and coordinates, leaving parameters and other functions unchanged (the coordinate of the functions however will be discretized). The result is by default a VDE type. To return a the finite difference expression in VCE form, the optional input `discretized` should be disabled:

```
VCE::Gen_Sten(expr,discretized=false)
```

Note: In the examples in the rest of this manual, we assume that the FD initialization is invoked and `f` and `g` are grid functions:

```
> read "FD.mpl": MFD():
Warning, grid_functions is not assigned
FD table updated, see the content using SFDT() command
> grid_functions:={f,g}:
```

Here is an example of discretizing differential expressions:

```
> A:=diff(f(x,y),x,y):
> B:=Gen_Sten(A);
          -f(i - 1, j - 1) + f(i - 1, j + 1) + f(i + 1, j - 1) - f(i + 1, j + 1)
 B := -1/4 ------------------------------------------------------------------------
                                        hy hx
 > Gen_Sten(diff(f(x),x)+g(y)+cos(f(x))+r(x)+z);
     f(i - 1) - f(i + 1)
-1/2 -------------------- + g(j) + cos(f(i)) + r(x(i)) + z(k)
              hx
 > Gen_Sten(A,discretized=false);
    -f(x - hx, y - hy) + f(x - hx, y + hy) + f(x + hx, y - hy) - f(x + hx, y + hy)
 -1/4 ---------------------------------------------------------------------------
                                    hy hx
```

Example 5: Discretizing a PDE

As one can see, the default discretization scheme in FD is centered (and second order accurate). In the next section, we describe how to change the finite difference scheme.

4.2 Discretization Scheme, `FD_table`

FD uses an internal table, `FD_table`, to perform the finite difference operations such as ones in Example 5. This table, simply is a list of the points that can be used for the n'th derivative computation for each of the coordinates `(t,x,y,z)`. For example, the `x` compoent of this table is:

```
> FD_table[x];
[[0], [-1, 0, 1], [-1, 0, 1], [-2, -1, 0, 1, 2], [-2, -1, 0, 1, 2], ...
```

where n'th element (counting from zero), is a list of points specifiying the finite differencing scheme for the n'th derivative along `x`. The numbers present the list of neighbooring points to `x(i)` that are allowed to be used for FDA. For instance, the third element, `[-2,-1,0,1,2]`, presents the 5 points: centeral point `x(i)`, 2 to left and 2 to right, that are allowed for FDA of the third derivatives in `x` coordinate. This is demonstrated in the following diagram.

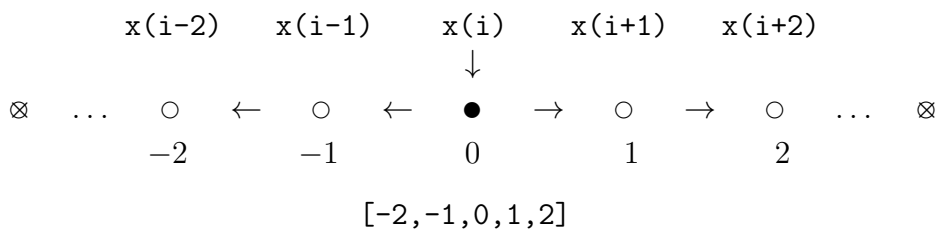


Figure 1: Five points specifing the FDA scheme for the third derivatives in `FD_table` in `x` direction.

FD initializes the finite difference table when `Make_FD()` is invoked. By default, the table is upto the 5'th derivatives (adjustable by the global variable `MAX_DERIVATIVE_NUMBER=5`) in all dimensions, and the points expand symmetrically around the central point (centered finite differencing).

4.3 Changing the FDA Scheme: `FDS`, `Update_FD_Table`

The FD scheme can be chosen by adjusting the content of `FD_table`. FD provides a convenient routine for this purpose:

```
Update_FD_Table(order::integer,fds::FDS);
```

in which the user specifies the desired order of accuracy, `order`, and the scheme via the second argument fds. This argument is a table with a particular format which we refer as a *Finite Difference Specifier* (FDS). A FDS is a table for the 4 coordinates, `(t,x,y,z)`,

```
fds:=table( [ t=... , x=..., y=... , z=...] );
```

and each element has the following format:

```
X = [p_left,-1] or [-1,-1] or [-1,p_right]
```

in which `X` denotes one of the coordinates, and the values `p_left` and `p_right` are known integers. `p_left` specifies how many points to left of the central point is allowed, and similarly `p_right` specifies the number of points to the right that can be used in an FDA for coordinate `X`. If these values are set to -1 it allows FD to expand in that direction to as many point as needed to achieve the desired accuracy. At least one of the p-values must be set to -1. Particularly, the `p_left` and `p_right` need to be adjusted for creating FDAs that can be applied in the vicinity of the boundaries of the numerical grid. This is demonstrated in the following diagram:

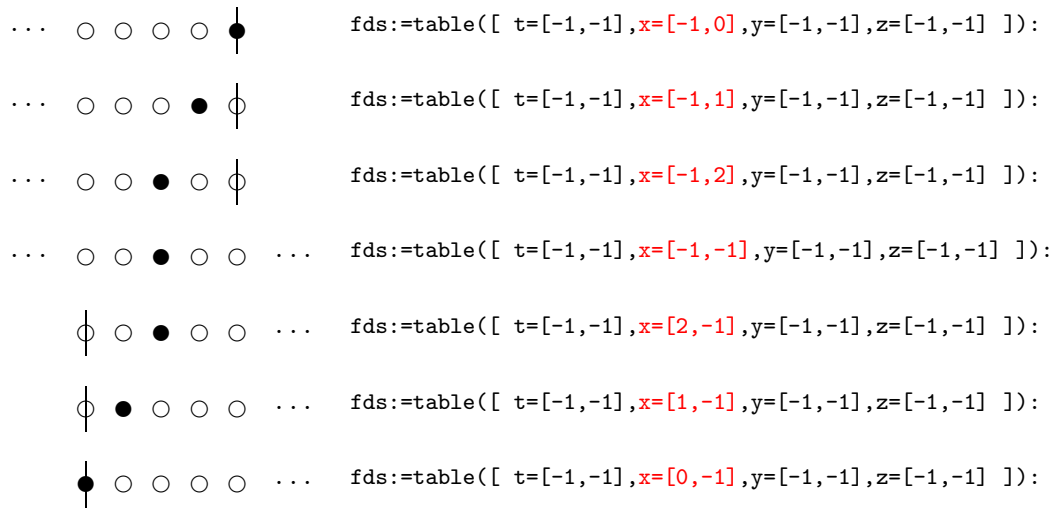


Figure 2: Specifying different types of FD schemes: note the values in the highlighted color and how it associates with each case at the vicinity of the boundary in x direction.

We remind the reader that higher derivatives require more points. In addition, increasing the accuracy `order` also adds to the number of the points used in FDAs. The routine `Update_FD_Table` has a built-in function $P(n,m)$

$$\frac{\partial^m}{\partial X^m} \text{ with } O(h^n) \text{ accuracy} \rightarrow P(n,m) \tag{66}$$

for each of the forward, backward and centered schemes that estimates the minimum number of points required to achieve the desired accuracy (or better).

For example the following code updates the FD table use FD scheme forward in time, centered in `x`, backward in `y` and asymetric backward in `z`, with 4'th order accuracy. The resulting `FD_table` is demonstrated by inspecting each element of it:

```
> fds:=table([t=[0,-1],x=[-1,-1],y=[-1,0],z=[-1,2]]):
> Update_FD_Table(4,fds):
FD table updated, see the content using SFDT() command
> FD_table[t];
[[0], [0, 1, 2, 3, 4], [0, 1, 2, 3, 4, 5, 6],...]
> FD_table[y];
[[0], [-4, -3, -2, -1, 0], [-6, -5, -4, -3, -2, -1, 0], ...]
> FD_table[z];
[[0], [-2, -1, 0, 1, 2], [-4, -3, -2, -1, 0, 1, 2], [-4, -3, -2, -1, 0, 1, 2],...]
```

Example 6: Changing the Finite Difference Scheme

We note that FD table can be updated manually by overwriting the elements, however this method is error-prone, and higher derivatives in particular might not have a sufficient number of points to be evaluated as a FDA. For example, in the following, we specify only 2 points for the second derivative in time, and the `Gen_Sten` procedure outputs an error as it is impossible to compute the FDA equivalent of the input according to the FD table:

```
> FD_table[t]:=[[0],[0,1,2],[0,1]]:
> Gen_Sten(diff(f(t,x),t));
           -f(n, i) + f(n + 1, i)
           ----------------------
                    ht
> Gen_Sten(diff(f(t,x),t,t));
Error, (in Calc_Stencil_L) Failed to find FDA coefficients, check FD_table content!
```

Finally, we note that the entire content of `FD_table` (rather lengthy sequence of integers!) can be viewed using the procedure:

```
Show_FD_Table();
```

4.4 Accessing the FD Results: `Show_FD`

If the `Gen_Sten` procedure is used to perform finite differencing on a lengthy differential expression, the resulting FDA is not human readible. To better present what `Gen_Sten` has performed, the routine stores the differential expressions it finds in the input and their FDA equivalent that it replaces them with, in an internal table named `FD_results`. The content of this table can be accessed using the procedure:

```
Show_FD();
```

For example, consider the following finite differencing operation:

```
> A:=diff(y*f(x,y)*diff(sin(x*y)*g(x),x),x,y):
> B:=Gen_Sten(A):
memory used=11.4MB, alloc=5.4MB, time=0.59
> lprint(B);

1/2*(-f(i-1,j)+f(i+1,j))/hx*(cos(x(i)*y(j))*y(j)*g(i)-1/2*sin(x(i)*y(j))*(g(i-1)-g(i+1))
```

```
/hx)+1/4*y(j)*(f(i-1,j-1)-f(i-1,j+1)-f(i+1,j-1)+f(i+1,j+1))/hy/hx*(cos(x(i)*y(j))*y(j)*g
(i)-1/2*sin(x(i)*y(j))*(g(i-1)-g(i+1))/hx)+1/2*y(j)*(-f(i-1,j)+f(i+1,j))/hx*(-sin(x(i)*y
(j))*x(i)*y(j)*g(i)+cos(x(i)*y(j))*g(i)-1/2*cos(x(i)*y(j))*x(i)*(g(i-1)-g(i+1))/hx)+f(i,
j)*(-sin(x(i)*y(j))*y(j)^2*g(i)-cos(x(i)*y(j))*y(j)*(g(i-1)-g(i+1))/hx+sin(x(i)*y(j))*(g
(i-1)-2*g(i)+g(i+1))/hx^2)+1/2*y(j)*(-f(i,j-1)+f(i,j+1))/hy*(-sin(x(i)*y(j))*y(j)^2*g(i)
-cos(x(i)*y(j))*y(j)*(g(i-1)-g(i+1))/hx+sin(x(i)*y(j))*(g(i-1)-2*g(i)+g(i+1))/hx^2)+y(j)
*f(i,j)*(-cos(x(i)*y(j))*x(i)*y(j)^2*g(i)-2*sin(x(i)*y(j))*y(j)*g(i)-sin(x(i)*y(j))*x(i)
*y(j)*(-g(i-1)+g(i+1))/hx+cos(x(i)*y(j))*(-g(i-1)+g(i+1))/hx+cos(x(i)*y(j))*x(i)*(g(i-1)
-2*g(i)+g(i+1))/hx^2)

# Checking if B is indeed an FDA for A:
> E:=DtoC(B):
> E:=convert(series(E,hx,4),polynom):
> E:=convert(series(E,hy,4),polynom):
> residual:=simplify(eval(A-E,hx=0,hy=0));
                 residual := 0
```

Expression `A` has several derivatives of the functions `f` and `g` that are replaced with FDA expressions. Now by invoking `Show_FD()` we can see what replacements have been done:

```
> Show_FD();

 d                 -f(i - 1, j) + f(i + 1, j)
{-- f(x, y) = [1/2 --------------------------, [[x, 2], [y, -1]]],
 dx                           hx

 d                 f(i, j - 1) - f(i, j + 1)
 -- f(x, y) = [-1/2 --------------------------, [[y, 2], [x, -1]]],
 dy                           hy

 d              -g(i - 1) + g(i + 1)
 -- g(x) = [1/2 --------------------, [[x, 2]]],
 dx                     hx

  2
 d           g(i - 1) - 2 g(i) + g(i + 1)
 --- g(x) = [---------------------------, [[x, 2]]],
   2                      2
 dx                     hx

 d               g(j - 1) - g(j + 1)              d
 -- g(y) = [-1/2 -------------------, [[y, 2]]], ----- f(x, y) = [
 dy                     hy                     dy dx

      -f(i - 1, j - 1) + f(i - 1, j + 1) + f(i + 1, j - 1) - f(i + 1, j + 1)
 -1/4 ------------------------------------------------------------------------,
                                    hy hx
 [[x, 2], [y, 2]]] }
```

Here the numbers next to the coordinate variables `x,y` denotes the order of accuracy of the replacement, and as expected they are all second order accurate. -1 represents exact FDA, i.e. there is no differentiation with respect to that coordinate. Note that this accuracy is *not* what user specifies when updating FD scheme (in previous section). It is indeed the computed value of the actual accuracy of FDA which

should be equal or higher to the user specified value.

4.5 Defining Manual Finite Difference Operators: FD

FD provides a way to define an arbitrary FDA operator. In principal, any finite difference operator can be created from the shifting operator (See [7]) defined (in 1 dimension) as:

$$E(f_i) = f_{i+1} \tag{67}$$

and its inverse is simply: $E^{-1}(f_i) = f_{i-1}$. The generalizaion of this operator is defined in the FD toolkit, and is named `FD` with the following format:

```
VDE::FD(dexpr::VDE, [ [t_shift] ,[x_shift,y_shift,z_shift] ])
```

in which `FD` takes an input `dexpr` of type VDE, and returns a VDE that is shifted by the given integers `(t_shift, x_shift,y_shift,z_shift)`. If there is no time index dependency in the expression, the first argument, `[t_shift]`, can be dropped and the routine accepts a shorter format:

```
FD(VDE,[x_shift,y_shift,z_shift])
```

Similarly if `z` index `k` does not occur in the VDE, the routine accepts shorter list `[x_shift,y_shift]` and so on. For example, the following demonstrates the definition of 3 manual FDA operators: 1) a forward time derivative FDA (`DT`) that is equivalent to ∂_t upto first order accuracy, 2) centered in x derivative FDA (`DXC`), which is equivalent to ∂_x upto second order accuracy, and 3) the time averaging operator `AVGT` that is *not* an FDA. This operator is usually used in Crank-Nicolson method to create a implicit FD scheme.

```
> DT := f -> ( FD(f,[[1],[0]]) - FD(f,[[0],[0]]) )/ht:
> df:= DT(f(n,i));
                        f(n + 1, i) - f(n, i)
                 df := ---------------------
                                 ht
> DXC:= f -> ( FD(f,[1,0]) - FD(f,[-1,0]) ) /(2*hx):
> DXC(f(i)*x(i)^2*g(j)+y(j));
                                    2                          2
                   f(i + 1) x(i + 1)  g(j) - f(i - 1) x(i - 1)  g(j)
               1/2 ---------------------------------------------------
                                          hx
> AVGT := f -> ( FD(f,[[1],[0]]) + FD(f,[[0],[0]]) )/2:
> AVGT(Gen_Sten(diff(f(t,x),x)));
          f(n + 1, i - 1) - f(n + 1, i + 1)       f(n, i - 1) - f(n, i + 1)
     -1/4 --------------------------------- - 1/4 -------------------------
                          hx                                 hx
```

Example 7: Defining manual dinite difference operators

5 Posing a PDE & Boundary Conditions over a Discrete Domain

In solving PDEs, it often occurs that some part of the discretized domain needs special treatment. By its nature, boundary points require different equations than the original PDE. In adddition, if the discretization scheme results in large finite difference molecules, the points next to the boundaries also require special handling. For example consider 4'th order accurate FDA of the derivative of a function, $\partial_x f(x)$:

```
                    f(i - 2) - 8 f(i - 1) + 8 f(i + 1) - f(i + 2)
              1/12 ----------------------------------------------
                                          hx
```

This expression cannot be evaluated where $i < 3$ or $i > N_x - 2$, as the finite difference molecule `(-2,-1,0,1,2)` require points that do not exist in the discretized domain at these limits. In this section, we describe the methodology to create different equations for each part of the numerical domain, and the facilities FD provides to impose boundary conditions and implement techniques such as ghost cells.

5.1 Discrete Domain Specifier: `DDS`

To specify each portion of the discrete domain, $\{i \in (1, N_x)\} \times \{j \in (1, N_y)\} \cdots$, FD uses a syntax similar to RNPL [8], via a derived data type that we refer as Discrete Domain Specifier (DDS). A DDS is a list of equations:

```
DDS = [ equation1, equation2, ...  ]
```

where each equation specifies part of the discrete domain and has the following LHS and RHS:

```
each equation:  { indexeq1, indexeq2, ...  } = expression
```

in which each `expression` can be a VDE, or a continuous PDE, and each `indexeq` describes the indexing for one of the spatial dimensions:

```
each indexeq:  I = [start,NI-stop,step]
```

Here, the variable `I` denotes one of the indexing labels, `(i,j,k)`, `NI` is the associated domain size `Nx,Ny,Nz`, and `step` is a known integer that determines the stepping size. The `indexeq` symbolizes a portion of the domain in which index `I` takes the values: `(start,start+step,start+2*step,...)` and ends at value smaller or equal to `NI-stop`. The reader may notice that this is exactly equivalent to a *for loop* structure. For example

```
{ i = [1,Nx,1] , j =[2,Ny-1,2] } = ...
```

is equivalent to (in Fortran syntax):

```
DO i=1,Nx,1
  DO j=2,Ny-1,2
    ...
  ENDDO
ENDDO
```

The following example clarifies this syntax, and demonstrates a DDS for heat equation where the boundary points are fixed to values `T0` and `T1` and interior points are specified by the heat equation.

```
HeatEq:= diff(f(t,x),t) - diff(f(t,x),x,x);
HeatDDS := [
  { i=[1,1,1]     } = f(n+1,i) - T0 + myzero*x(i)   ,
  { i=[2,Nx-1,1]  } = Gen_Sten(HeatEq)              ,
  { i=[Nx,Nx,1]   } = f(n+1,i) - T1 +myzero*x(i)
];
```

Example 8: 1-D discrete domain specifier for the heat equation

The necessity of `myzero*x(i)` expression will become clear later when we use this DDS as an input to FD's solver routine generator.

Note that heat equation and its boundary conditions are simple and compact enough to be discretized inside the DDS. For a more complex case, it is better to create the discrete version of the equations for the boundaries seperaterly, and pass them into the DDS using human readable names. For example, the following demonstrates a 2 dimensional DDS where each boundary uses a specific discrete equation priorly created by the user:

```
mydds2d := [
 # Interior points:
   { i=[2,Nx-1,1] , j = [2,Ny-1,1] } =  EQD_interior ,
 # Boundaries:
   { i=[1,1,1]    , j = [1,Ny,1]   } =  EQD_left     ,
   { i=[Nx,Nx,1]  , j=[1,Ny,1]     } =  EQD_right    ,
   { i=[1,Nx,1]   , j=[1,1,1]      } =  EQD_bottom   ,
   { i=[1,Nx,1]   , j=[Ny,Ny,1]    } =  EQD_top
];
```

Example 9: Two dimensional DDS

For a set of coupled PDEs, the user can create the FDAs and DDS's using a Maple foor loop. Note that FD will check for consistency of the LHS and RHS of each element of DDS as well as the consistency between all the elements. It will raise errors if the finite difference expression on the RHS does not have the same dimensionality as the LHS. However at the moment FD does *not* check if the finite difference molecule on the RHS fits into the domain specified on the LHS. The user need to be careful with the manual discretization of the equations, and to avoid out of range errors, it is best to use finite difference specifiers (FDS) discussed in Sec 4.3.

5.2 Imposing Outer Boundary Conditions

The next step is to create the appropriate FDA expressions (the RHS expressions in the DDS) that are compatible with specfic boundary conditions and also are created under consideration that there are limitations on the allowed points in the vicinity of the boundary points. The case of fixing the value of the function or *Dirichlet boundary condition* is quite simple and demonstrated in the example for heat equation. Often other types of boundary conditions appear in physical systems. One of particular interest is the "out-going" type or *Neumann boundary condition*. For a 1-D wave equation the out-going boundary condition is given by:

$$\partial_t f(t,x) = -\partial_x f(t,x) \tag{68}$$

for the right side boundary `i=Nx` that corresponds to the approximate positive "infinity" of the numerical domain $x = +L_\infty$. The out-going boundary condition at the the left side of the numerical domain is given by:

$$\partial_t f(t,x) = +\partial_x f(t,x) \tag{69}$$

for the point `i=1` or $x = -L_\infty$. To implement such boundary conditions, one needs to use FDA expressions that can be evaluated at the point of boundary that does not allow symmetric FD scheme. As described in Sec. 4.3, this is achieved by changing the FDA scheme in FD using finite difference specifiers (FDS). For example, the following demonstrates an implementation of a mixed boundary for wave equation in which left boundary is fixed while the right boundary is outgoing. Note the change of FDA scheme using the FDS: `fds_backwardx`.

```
WaveEq := diff(f(t,x),t,t) - diff(f(t,x),x,x):
WaveEqBdy := diff(f(t,x),t) + diff(f(t,x),x):

WaveEqD := Gen_Sten(WaveEq):
```

```
fds_backwardx:=table([ t=[-1,-1],x=[-1,0],y=[-1,-1],z=[-1,-1] ]):
Update_FD_Table(2,fds_backwardx):

WaveEqBdyD := Gen_Sten(WaveEqBdy):

ddsWAVE:= [
   i=[1,1,1]      = f(n+1,i) - myzero*x(i)  ,
   i=[2,Nx-1,1]   = WaveEqD,
   i=[Nx,Nx,1]    = WaveEqBdyD
];
```

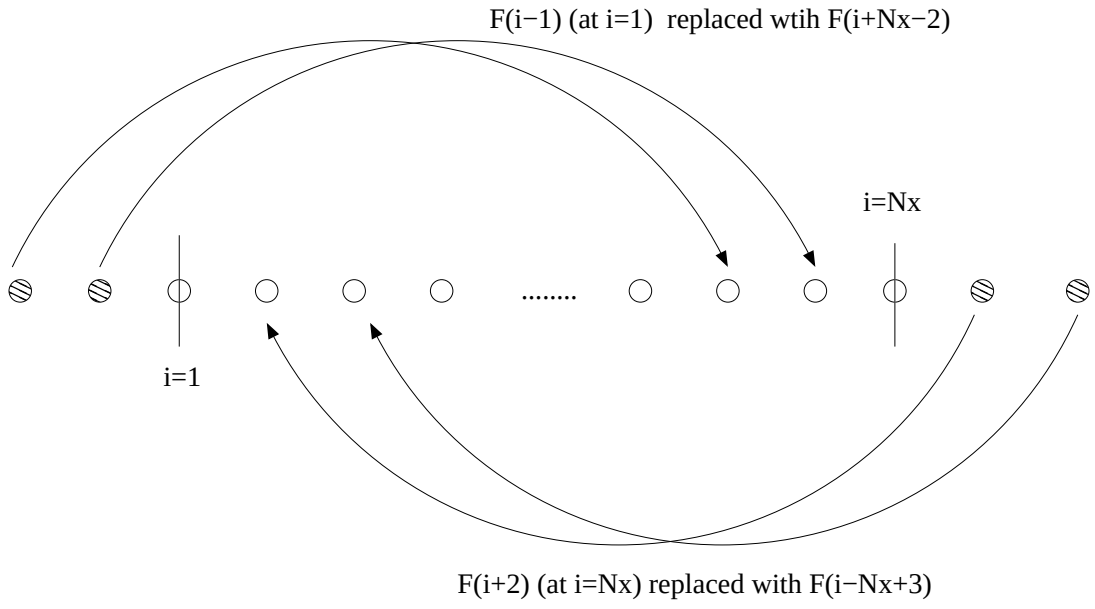
Example 10: Specifiying outgoing/mixed boundary condition for wave equation

5.3 Periodic Boundary Condition: `FD_Periodic`

Another common boundary specficiation is peridoc boundary condition (PBC). FD provides a facility to implement PBCs by making a VDE periodic. The procedure:

```
FD_Periodic(exprd::VDE,{I=1/NI})
```

takes an input, `exprd`, of type VDE and creates a periodic version of it. This location is specified by the second argument, in which `I` is one of the indeces `(i,j,k)` and the RHS is either 1 or `NI` where `NI` is one of the associated grid size `(Nx,Ny,Nz)`. For example `i=1` denotes that a periodic version of VDE is needed at the left boundary and `i=Nx` denotes the same for the right boundary point. The replacements done on FDA is illustrated in the following graph:



The following example, demonstrates the effect of the `FD_Periodic` procedure on a VDE:

```
> FD_table[x]:=[ [0], [-1,0,1] ,[-2,-1,0,1,2] ]:
> A:= Gen_Sten(diff(f(x),x,x));
                 f(i - 2) - 16 f(i - 1) + 30 f(i) - 16 f(i + 1) + f(i + 2)
      A := -1/12 ----------------------------------------------------------
                                          2
```

```
                                                    hx
> FD_Periodic(A,{i=1});
          f(i - 3 + Nx) - 16 f(i - 2 + Nx) + 30 f(i) - 16 f(i + 1) + f(i + 2)
    -1/12 ------------------------------------------------------------------
                                                    2
                                                   hx
> FD_Periodic(A,{i=Nx});
          f(i - 2) - 16 f(i - 1) + 30 f(i) - 16 f(i + 2 - Nx) + f(i + 3 - Nx)
    -1/12 ------------------------------------------------------------------
                                                    2
                                                   hx
```

Finally, using this procedure, the implementation of a periodic DDS for wave equation can be achieved as following:

```
ddsWAVE_Periodic:= [
  { i=[1,1,1]     } = FD_Periodic(WaveEqD,{i=1})  ,
  { i=[2,Nx-1,1]  } = WaveEqD,
  { i=[Nx,Nx,1]   } = FD_Periodic(WaveEqD,{i=Nx})
];
```

Example 11: Implementation of a periodic boundary condition

in which `WaveEqD` is the same as Example 10.

5.4 Implementing Ghost Cells for Odd and Even Functions: `A_FD_Odd`, `A_FD_Even`

The boundaries of the numerical domain often correspond to the spatial infinity. However, a different coordinate system than cartesian coordinate can be chosen, particularly to impose a certain symmetry. For example, one can work in a spherical coordinate and assume that the function's spatial dependency is only of the form:

$$f(t,x,y,z) = f(t,r) \quad , \quad r = \sqrt{x^2+y^2+z^2}\,. \tag{70}$$

In this case, the domain of the PDE (and the function f) is $r \in (0,\infty)$. The point $r=0$ is superficially a boundary of the numerical domain in this coordinate system, while in fact there is no physical boundary. These types of boundaries are often referred as *inner boundaries* and usually are treated by imposing a specific behaviour for the functions derived from the underlying symmetry.

One common scenario that occurs in the point (or axis) of symmetry is that functions (depending on what they represent: scalar, vector, compoent of a tensor etc) become even or odd. For example, a scalar function with spherical symmetry, $\psi(t,r)$, is an even function at $r=0$, i.e:

$$\psi(t,-r) = \psi(t,r) \tag{71}$$

Note that here, $-r$ is neither a physical location, nor is part of the numerical domain. However, one can simply consider the function along the x axis (where $r=|x|$) and the refection symmetry $x \to -x$ implies that the function is even in x. This means, equivalently, function is even in r if we consider an extension of it to $r<0$ that represents the value of the function at $-x$. More rigorously, the functions at the limit of $r \to 0$ take one of the two forms:

$$f(t,r) = C_0(t) + C_2(t)r^2 + C_4(t)r^4 + \ldots \quad \to \quad \text{function is even} \tag{72}$$

$$f(t,r) = C_1(t)r + C_3(t)r^3 + C_5(t)r^5 + \ldots \quad \to \quad \text{function is odd} \tag{73}$$

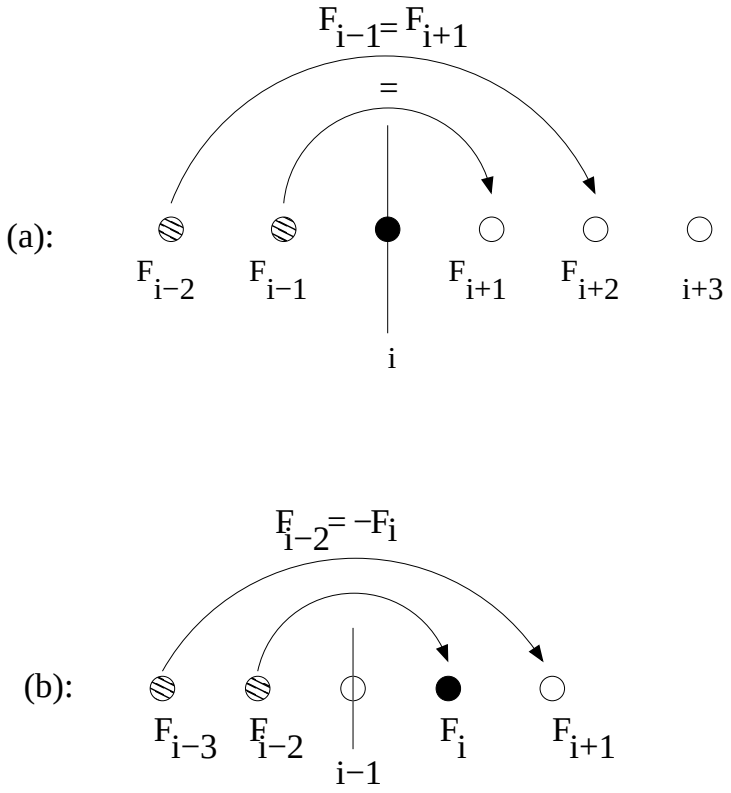
where the first case is for "scalar" functions and the second case is for "vector" functions.

This property of the functions at inner boundaries allows a discretization technique known as "ghost cells" in finite difference method. For example, consider the second and first derivative of the function with 4'th order accuracy:

```
# FD Updated to 4'th order before...
> A:=Gen_Sten(diff(f(x),x,x));
                    f(i - 2) - 16 f(i - 1) + 30 f(i) - 16 f(i + 1) + f(i + 2)
        A := -1/12 ------------------------------------------------------------
                                              2
                                             hx
> B:=Gen_Sten(diff(f(x),x));
                              f(i - 2) - 8 f(i - 1) + 8 f(i + 1) - f(i + 2)
                  B := 1/12 ---------------------------------------------
                                              hx
```

Obviously, these terms cannot be used at $i = 1$, the left boundary point, and also the point next to it $i = 2$. However, if we impose the even or odd behaviour on the function, the values `f(i-1)` and `f(i-2)` are known from the symmetry. For example, assuming that `i` is the point of symmetry, i.e the FDA will be used at `i=1`, then for an even function: `f(i-1) = f(i+1)`. This condition is illustrated in the following diagram (a). Similarly, for an odd function we have: `f(i-2) = -f(i+2)`.

Consider another example where `f` is odd, and the FDA will be used at `i=2`, the point next to the inner boundary point. The out-of-bound term in the FDA in this case is only `f(i-2)` and from the symmetry we must have: `f(i-2) = -f(i)`. The following diagram (b) clarifies this condition:



One standard method to implement this symmetry is to actually extend the numerical domain to have extra points outside the physical domain. These points, namely *ghost cells*, are updated via the symmetry, and allow FDA operations at the boundary point.

FD provides a tool equivalent to the ghost cell technique. One can directly manipulate the FDA

expression according to the symmetry such that the out of bound terms are replaced appropriately and the FDA can be used at the boundary points. FD provides two procedures to perform this task:

```
A_FD_Even(exprd::VDE,coord,set_of_even_funcs,symm_loc,"forward/backward")
```

```
A_FD_Odd(exprd::VDE,coord,set_of_odd_funcs,symm_loc,"forward/backward")
```

where `exprd` is an FDA expression of type VDE, `coord` is the name of the coordinate which we are imposing the symmetry on (one of the `(x,y,z)`), the two variables `set_of_even_funcs` and `set_of_odd_funcs` are of type set and include the name of the functions that are even and odd respectively. `symm_loc` is an integer that determines the location of the inner boundary relative to the point where FDA will be evaluated. For example the diagram (a) above corresponds to: `symm_loc = 0` and the diagram (b) can be imposed by setting: `symm_loc = -1`. The last argument is of type string, and determines if the replacement should be "forward" – when the smaller index values are the out-of-bound ones and must be replaced – or "backward", i.e the larger index values are the out-of-bound and require replacement with indexed terms inside the physical domain. Normally, if the inner boundary is chosen to be the index $i = 1$ or ($j = 1, k = 1$ in higher dimensions), these procedures will only be use in "forward" mode.

The following demonstrates the usage of these two procedures and their output:

```
> A:=Gen_Sten(diff(f(x),x,x));
                    f(i - 2) - 16 f(i - 1) + 30 f(i) - 16 f(i + 1) + f(i + 2)
        A := -1/12 ------------------------------------------------------------
                                              2
                                             hx
# Diagram (a) above:
> A_FD_Even(A,x,{f},0,"forward");
                                    2 f(i + 2) - 32 f(i + 1) + 30 f(i)
                           -1/12 ----------------------------------
                                                2
                                               hx
# Diagram (b) above:
> A_FD_Even(A,x,{f},-1,"forward");
                               31 f(i) - 16 f(i - 1) - 16 f(i + 1) + f(i + 2)
                      -1/12 ---------------------------------------------
                                                2
                                               hx
> B:= Gen_Sten(diff(f(x),x));
                         f(i - 2) - 8 f(i - 1) + 8 f(i + 1) - f(i + 2)
             B := 1/12 ---------------------------------------------
                                             hx
> A_FD_Odd(B,x,{f},0,"forward");
                               -2 f(i + 2) + 16 f(i + 1)
                        1/12 -------------------------
                                          hx
> A_FD_Even(B,x,{f},0,"forward");
                                        0
```

Example 12: Imposing even and odd symmetry at inner boundary point

Note that in the last execution, the result is identical to zero since the first derivative of an even function is zero at the point of symmetry. We also note that if the FDA involves several functions of mixed even and odd type, both of the routines need to be applied consecutively to the FDA to achieve a proper discretized version, usable at the inner boundary point.

6 Solving a PDEs

This section demonstrates how to incorporate all of FD's procedures and structures to solve a PDE.

6.1 Creating Initializer Routines: `Gen_Eval_Code`

The first step is to create routines that initialize the function $f(t=0,x,y,z)$. If this initialization has an explicit function form depending on the coordinate and can be evaluated on every point of the numerical grid `(x(i),y(j),z(k))` then it can be simply created using the procedure:

```
Gen_Eval_Code(expr,input="c*/d",proc_name="my_init_proc");
```

where `expr` is either a continuous expression (setting `input="c"`, this is the default setting) or it is a VDE (by setting `input="d"`). The next option `proc_name` is the name of the Fortran procedure we want to create and it denotes both the name of the file (without the suffix `.f`) and the name of the procedure.

For example, consider the case where we want to set the inital profile of the wave package to a Gaussian function:

$$f(t=0,x,y) = A\exp\left(-\frac{(x-x_c)^2}{\delta_x^2} - \frac{(y-y_c)^2}{\delta_y^2}\right) \tag{74}$$

the following FD code performs the desired task:

```
> read "../FD.mpl": MFD():
Warning, grid_functions is not assigned
FD table updated, see the content using SFDT() command
> grid_functions:={f}:
> init_f:=A*exp( -(x-xc)^2/delx^2 - (y-yc)^2/dely^2 ):
> Gen_Eval_Code(init_f,input="c",proc_name="init_to_gauss");
Fortran Code is written to init_to_gauss.f
C header is written to init_to_gauss.h
C call is written to init_to_gauss_call
```

Example 13: Creating Initializer Fortran routines

Similar to the very first example of creating IRE routines, all of FD's code generator routines create 3 files, `X.f`, `X.h` and `X_call`, where the Fortran file `X.f` is the body of the Fortran procedure that performs the desired task. All of the procedures generated by FD have a last argument named **res**. For examle the routine created by the execution above, `init_to_gauss.f` has the following header:

```
subroutine init_to_gauss(x,y,Nx,Ny,A,delx,dely,xc,yc, res)
```

in which the highlighted `res` is the pointer to the vector that stores the returned value of the procedure. In this case it is the function. Therefore user should pass in the pointer that stores `f` at inital time in the driver code. The header file `.h` is a wrapper that can be included in a C driver program to use this routine. In the example above, the content of the file, `init_to_gauss.h` is:

```
void init_to_gauss_(double *x,double *y,int *Nx,int *Ny,double *A,double *delx,
double *dely,double *xc,double *yc,double *res);
```

and finally the `X_call` files are typicall C calls that can be copied to the C driver and after changing the last argument **res** to the appropriate pointer, can be used to call the Fortran routine. In the example above, the content of `init_to_gauss_call` is:

```
init_to_gauss_(x,y,&Nx,&Ny,&A,&delx,&dely,&xc,&yc,res);
```

We note that if the expression that is passed to the procedure contains derivatives, (or FDA expressions in discrete form) then this procedure only evaluates/initializes the expression at the points where the evaluation is possible i. e. allowed by the size of the finite difference molecule (FDM). This usually results in a Fortran routine that ignores the evaluation of the function on the boundary points (and perhaps in its vicinity depending on how large the resulting FDM is). If the evaluation is required at the boundary points, then the procedure described in the next section should be used.

6.2 Point-wise Evaluator Routines with DDS: A_Gen_Eval_Code

If the initialization is needed to vary at different portions of the discrete domain, the Fortran routine can be generated using the "evaluator" routine generator:

```
A_Gen_Eval_Code(dds:DDS,input="c*/d",proc_name="my_eval_proc");
```

where the only difference between this procedure and `Gen_Eval_Code` is in the first argument, where this procedure accepts `DDS` type to allow specific calculations at different parts of the domain. This procedure can also be used to evaluate a specific function that depends on the primary dynamical fields and their derivatives. It can also be used to evaluate the point-wise residuals of PDEs if needed.

For example, consider the problem where we want to evaluate the function f that is the laplacian of the function ϕ in cylenderical coordinate with axial symmetry:

$$f(\rho,z) = \nabla^2\phi = \frac{1}{\rho}\partial_\rho(\rho\partial_\rho\phi(\rho,z)) + \partial_z^2\phi(\rho,z) = \partial_\rho^2\phi + \frac{\partial_\rho\phi}{\rho} + \partial_z^2\phi \tag{75}$$

Note that we would like to evaluate this laplacian value on the axis $\rho = 0$ (which is an inner boundary) as well as the interior points. To do so, we need to deal with the irregular term $\frac{1}{\rho}$ and also impose an inner boundary condition at $\rho = 0$. As discussed previously, these types of inner boundary conditions are dealt by looking into the behaviour of the function at the limit of approaching the boundary, here: $\rho \to 0$. We know that the function ϕ is a scalar and its first derivative $\partial_\rho\phi$ approaches zero on the axis as $O(\rho)$. Using the L'Hospital's rule:

$$\lim_{\rho\to 0}\frac{\partial_\rho\phi}{\rho} = \frac{\partial^2\phi}{\partial\rho^2} \tag{76}$$

Therefore, two versions of the expression are used to evaluate f:

$$f = \nabla^2\phi = \begin{cases} \partial_\rho^2\phi + \frac{\partial_\rho\phi}{\rho} + \partial_z^2\phi & \text{if } \rho \neq 0 \\ 2\partial_\rho^2\phi + \partial_z^2\phi & \text{if } \rho = 0 \end{cases} \tag{77}$$

In addition, the evaluation of the derivative as an FDA at $\rho =$ requires implementation of boundary condition as described in Sec. 5.4. Here the inner boundary condition is created using the fact that ϕ is an even function in ρ. The following example demonstrates all of the steps described to achieve this evaluation:

```
read "../FD.mpl": CFD(): MFD():
grid_functions:={phi}:

Laplace_Interiour:= diff(phi(x,z),x,x) + diff(phi(x,z),x)/x + diff(phi(x,z),z,z):
Laplace_Boundary_D:= Gen_Sten(2*diff(phi(x,z),x,x) + diff(phi(x,z),z,z)):

dds_2Dlaplace:= [
{ i=[2,Nx-1,1] , k=[2,Nz-1,1] } = Gen_Sten(Laplace_Interiour),
{ i=[1,1,1], k = [2,Nz-1,1] } = A_FD_Even(Laplace_Boundary_D,x,{phi},0,"forward"),
{ i=[Nx,Nx,1] , k=[1,Nz,1] } = myzero*x(i)*z(k),
{ i=[1,Nx,1] , k =[1,1,1] } = myzero*x(i)*z(k),
{ i=[1,Nx,1] , k =[Nz,Nz,1] } = myzero*x(i)*z(k)
]:
```

```
A_Gen_Eval_Code(dds_2Dlaplace,input="c",proc_name="eval_laplace");
Fortran Code is written to eval_laplace.f
C header is written to eval_laplace.h
C call is written to eval_laplace_call
```

Example 14: Point-wise Evaluator Routine Generator Using a DDS

6.3 Creating IRE Testing Routines: `Gen_Res_Code`

If the function that needs to be evaluated is indeed a residual, i.e. expected to be zero in the continuum limit, then often the user is interested in monitoring the l_2-norm of this residual. FD provides a procedure that creates a Fortran routine for such an evaluation:

```
Gen_Res_Code(expr,input="c*/d",proc_name="my_res_proc");
```

where `expr` can be a PDE residual in a continuous form or a VDE. The only difference between this procedure and `Gen_Eval_Code` is that the Fortran routine generated here will perform a l_2-norm (root mean square to be specific) on the function and returns a single real number. This routine can be used as a fast prototyping tool to create Independent Residual Evaluator routines. The following demonstrates an example of creating IRE for wave equation:

```
read "../FD.mpl": Clean_FD(): Make_FD():

grid_functions := {f}:

WaveEq := diff(f(t,x),t,t) = diff(f(t,x),x,x):

Gen_Res_Code(lhs(WaveEq)-rhs(WaveEq),input="c",proc_name="ire_wave");
```

Example 15: Fast Prototyping IRE Routines

6.4 Creating Piece-wise Residual Evaluator Routines: `A_Gen_Res_Code`

Similar to the generalization of `Gen_Eval_Code` to `A_Gen_Eval_Code` such that the procedure accepts a DDS such that the function can be evaluated on each portion of the discret domian, here `A_Gen_Res_Code` extends the capability of previous procedure `Gen_Res_Code` to evaluate the l_2-norm of the residual that is specified by a DDS:

```
A_Gen_Res_Code(dds:DDS,input="d/c*",proc_name="my_res_proc");
```

This procedure is perhaps most useful to evaluate the norm of the residual of the PDE under study. The returned norm of the residual can be compared to a *threshold value* to determine if the PDE is numerically solved after applying the solver routine (or after certain number of iterations of the solver routines are applied). Note that this routine can also be used as an IRE generator. Example 14 can be used to demonstrate the use of this procedure, the difference is that the Fortran routine created by this procedure will return the l_2-norm of the laplace equation, and therefore can be useful if we are monitoring the norm of the residual and convergence of our numerical solver.

6.5 Creating Solver Routine: `A_Gen_Solve_Code`

As we discussed in Sec. 2.2, for a given FDA of a PDE written in canonical form:

$$PDE = L(f) = 0 = L^h(f^h) \tag{78}$$

the solving process involves finding the unknowns f_{ijk} (for a boundary value problem) or f_{ijk}^{n+1} for initial value problem using f_{ijk}^{n}. As introduced in Sec. 2.2, a standard approach for a nonlinear system is to use Newton-Gauss-Seidel iterative method. FD provides a procedure that generates routines which implement single iteration of this method:

```
A_Gen_Solve_Code(dds:DDS,{solve_for_var},input="d/c*",proc_name="my_solver_proc");
```

where the first argument is of type `DDS`, and the second argment is a set of unknowns for which the FDA must be solved. At the moment this set must contain only a single term, such as `f(n+1,i,j,k)` as the unknown. The created Fortran routine performs a single iteration of Newton-Gauss-Seidel and returns the "updated" function in the last argument, namely `res` which shall be adjusted by the user. This completes all the necessary tools to create a set of solver routines for a PDE, and in the next section we put together all of the features of FD discussed to demonstrate an implementation of a solver system for 1-D wave equation using an implicit scheme. This example also demonstrates the use of this solver procedure.

Note on `myzero` Expression

As it has been seen at several points in this document, the user needs to implement constant functions or residual equations by adding a trivial VDE such as `myzero*x(i)*y(j)`. This is due to the fact that FD uses VDE's to figure out the dimensionality and dependencies of the PDEs, therefore if a single expression such as a constant number is given to FD's discretization routines, it has no way of finding the dimensionality of the problem. In particular, the common scenaro that the use of `myzero` is essential is when in the equation that needs to be solved the solution simplifies to a single constant or zero. For instance, in Example 10 we are imposing fixed boundary condition $f = 0$ at $x = 0$, therefore the residual of the equation (LHS of equatio in canonical form: $L(f) = 0$) is simply: f. However, the implementation of this residual has to be $f - myzero * x$, since if f is passed in as the residual, the solver VDE simplifies to 0, which has no valid dependency on any discrete index, {`i,j,k,n`}, to be understood by FD.

6.6 Communicating with Parallel Computing Infrastructure

Here we present a simple communication method with a parallelization infrastructure (FD adopts PAMR's [4] standard). To achieve this goal a vector of integer flags, `phys_bdy` is passed to the solver/evaluator routines in which the value 1 denotes that the boundary is a real physical boundary, therefore the boundary condition should be imposed, and the value 0 denotes that it is a boundary between CPUs and usually no calculation is required as the parallel frameworks often implement between CPU ghost cells for the distributed subdomains. These flags are invoked by setting the variable `b` to their associated names `xmin,xmax,...` as noted in table .(62) The following example demonstrates a DDS that implements boundary flags:

```
ddsfWave := [
  { i=[2,Nx-1,1] , j=[2,Ny-1,1]          } =  PDEWave_D,
  { i=[1,1,1]    , j=[1,Ny,1]   , b=xmin } =  f(n+1,i,j) - myzero*x(i)*y(j),
  { i=[Nx,Nx,1]  , j=[1,Ny,1]   , b=xmax } =  f(n+1,i,j) - myzero*x(i)*y(j),
  { i=[1,Nx,1]   , j=[1,1,1]    , b=ymin } =  f(n+1,i,j) - myzero*x(i)*y(j),
  { i=[1,Nx,1]   , j=[Ny,Ny,1]  , b=ymax } =  f(n+1,i,j) - myzero*x(i)*y(j)
];
```

We encourage the reader to look into the Fortran files that are created using this type of DDS to inspect how the `phys_bdy` flags are positioned in the file.

The tutorial: `FD/tutorials/wave2d_pamr_fixed_boundary` in the distribution package is an implementation of a parallel 2 dimenstional wave equation solver.

6.7 Example: Crank-Nicolson Implementation of Wave Equation

We complete this section by combining all of the tools we discussed to a single Maple script that creates a solver routine, residual evaluator and an independent residual evaluator as well as an initializer routine for the 1 dimensional wave equation. The wave equation is given by:

$$\partial_t^2 f(t,x) = \partial_x^2 f(t,x)\,, \tag{79}$$

and can be reduced to a first order system by defining f_t as:

$$f_t(t,x) \equiv \partial_t f(t,x) \tag{80}$$

$$\Rightarrow$$

$$\partial_t f(t,x) = f_t(t,x) \tag{81}$$

$$\partial_t f_t(t,x) = \partial_x^2 f(t,x) \tag{82}$$

Here we assume periodic boundary conditions Note that the example, first implements an IRE for the system using the original form of the wave equation and FD's default second order leap-frog scheme. After that, the FD scheme is updated to forwards in time, and by virtue of time averaging we achieve second order accuracy. It also demonstrate how to create initializer routines as well as residual evaluator routines to measure how accurate the PDE is solved.

```
read "../FD.mpl": Clean_FD(); Make_FD();
grid_functions := {f,f_t};

eq1 := diff(f(t,x),t) = f_t(t,x);
eq2 := diff(f_t(t,x),t) = diff(f(t,x),x,x);
eq3 := diff(f(t,x),t,t) = diff(f(t,x),x,x);

Gen_Res_Code(lhs(eq3)-rhs(eq3),input="c",proc_name="ire_f");

FD_table[t] := [[0],[0,1]];

AVGT := a -> (   FD( a,[ [1],[0] ]) + FD( a,[ [0],[0] ]) )/2;

eq1_D :=   Gen_Sten(lhs(eq1)) - AVGT(Gen_Sten(rhs(eq1)));
eq2_D :=   Gen_Sten(lhs(eq2)) - AVGT(Gen_Sten(rhs(eq2)));

init_f:=A*exp(-(x-x0)^2/delx^2);
init_f_t:=idsignum*diff(init_f,x);

Gen_Eval_Code(init_f,input="c",proc_name="init_f");
Gen_Eval_Code(init_f_t,input="c",proc_name="init_f_t");

dss_f:= [
  { i=[1,1,1]     } = FD_Periodic(eq1_D,{i=1}) ,
  { i=[2,Nx-1,1]  } = eq1_D,
  { i=[Nx,Nx,1]   } = FD_Periodic(eq1_D,{i=Nx})
  ];

dss_f_t:= [
  { i=[1,1,1]     } = FD_Periodic(eq2_D,{i=1}) ,
  { i=[2,Nx-1,1]  } = eq2_D,
  { i=[Nx,Nx,1]   } = FD_Periodic(eq2_D,{i=Nx})
```

```
];

A_Gen_Res_Code(dss_f,input="d",proc_name="res_f",is_periodic=true);
A_Gen_Res_Code(dss_f_t,input="d",proc_name="res_f_t",is_periodic=true);

A_Gen_Solve_Code(dss_f,{f(n+1,i)},input="d",proc_name="u_f",is_periodic=true);
A_Gen_Solve_Code(dss_f_t,{f_t(n+1,i)},input="d",proc_name="u_f_t",is_periodic=true);
```

Example 15: Implementation of Crank-Nicolson Scheme to Solve 1D Wave Eq. (79)

Note that several other complete examples are included in FD's distribution package in the directory `tutorials`, including: 2D wave equation in parallel, non-linear mixed boundary 1D wave equation, heat equation, and 2D wave equation in cylenderical coordinate with axial symmetry. All of the examples in this manual are also included in the distribution under `examples` directory.

Also see: `http://laplace.phas.ubc.ca/People/arman/FD_doc/tutorials.html` for detailed tutorials on how to use FD.

7 List of Abbreviations

BVE: Boundary Value Problem
DDS: Discrete Domain Specifier
FD: Finite Difference, also the name of the toolkit
FDA: Finite Difference Approximation
FDE: Finite Difference Equation
FDM: Finite Difference Molecule
FDS: Finite Difference Specifier
IVE: Initial Value Problem
LHS: Left Hand Side
ODE: Ordinary Differential Equation
PBC: Periodic Boundary Condition **PDE**: Partial Differential Equation
RHS: Right Hand Side
VCE: Valid Continuous Expression
VDE: Valid Discrete Expression

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