Proto Design Document

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1 Introduction

Proto is a lightweight library designed for efficient solution of differential equations on domains composed of unions of structured, logically rectangular grids. The goal of Proto is to provide a fluent, intuitive interface that separates the complexities of designing and scheduling an algorithm. As both the tools and applications of high performance computing become continuously more intricate, libraries such as Proto will become more and more necessary to efficiently solve problems in a timely manner.

2 Variables, Notation, and Syntax

In general, variables which refer to tokens in Proto are written using a monospaced font. Vector-like objects are written in lower-case **bold**, number types use black-board font (\mathbb{R}), and sets are written in math calligraphy font (\mathcal{S}). Occasionally words are typed in bold-face simply for **emphasis**.

Variable Name	Variable Definition
$oldsymbol{D}$ or DIM	Number of space dimensions
\mathbb{Z}^D	$oldsymbol{D} ext{-dimensional Space of Integers}$
B	Rectangular subset of \mathbb{Z}^D
Box(V)	Domain of multidimensional rectangular array V
$[m{l},m{h}]$	Box with low and high corners $(\boldsymbol{l}, \boldsymbol{h})$
$ lap{T}$	Space of numbers of type T
$\mid\mid i,j,k,r,s,t\dots$	Points in \mathbb{Z}^D
$oldsymbol{e}^d$	Unit vectors in direction d
$oldsymbol{u}$	Point in \mathbb{Z}^{D} all of whose entries are 1

3 Spatial Discretizations on Rectangular Grids

We approximate solutions to partial differential equations in terms of **data arrays**, i.e. discrete values defined over rectangular regions (Boxes) in \mathbb{Z}^{D} .

$$\phi: \mathbf{B} \to \mathcal{T} \text{ i.e., } \phi_i \in \mathcal{T}, i \in \mathbf{B} \subset \mathbb{Z}^D,$$
 (1)

$$\mathcal{T} = \mathcal{T}(C_1, \dots, C_n) = \{ t_{c_1, \dots, c_n} : t \in \mathbb{T}, c_i \in [1, \dots, C_i] \},$$
 (2)

where \mathbb{T} is one of the real numbers (\mathbb{R}), the complex numbers (\mathbb{C}), or the integers (\mathbb{Z}), and $\mathbf{B} = [\mathbf{l}, \mathbf{h}]$ is a rectangular subset of $\mathbb{Z}^{\mathbf{D}}$ with low and high corners \mathbf{l}, \mathbf{h} . Thus ϕ takes on values in a space of multidimensional arrays of \mathbb{T} s. While we could flatten this into a single array of dimension $\mathbf{D}+n$, we choose not to. This is because the different indices have different mathematical meanings. The Box indices represent a discretization of physical space, with those indices used to define difference approximations to derivatives. The indices in \mathcal{T} represent different components in some state space. A second difference is that the range of indices for the Boxes are computed at run time, whereas we will assume that the range of component indices for any given ϕ are known at compile time. Multidimensional arrays have the usual algebraic operations associated with them:

• Assignment. If ϕ , ψ are data arrays with the same value space \mathcal{T} , we define the assignment operator

$$\psi := \phi \text{ on } \mathbf{B}' \Leftrightarrow \psi_{\mathbf{i}} := \phi_{\mathbf{i}} , \mathbf{i} \in \mathbf{B}'$$
$$\mathbf{B}' \subseteq \operatorname{Box}(\phi) \cap \operatorname{Box}(\psi)$$

If the qualifier **on** ... is omitted, then the assignment is assumed to take place on $Box(\phi) \cap Box(\psi)$.

• Addition of two data arrays; multiplication of a data array by a scalar. If ϕ , ψ have the same value spaces, then $\phi + \psi$ is defined on $\text{Box}(\phi) \cap \text{Box}(\psi)$, with $(\psi + \phi)_i = \psi_i + \phi_i$. If $t \in \mathbb{T}$, then $(t\phi)_i = t\phi_i$.

A broad range of discretized PDE operators can be represented as the composition of **stencil** and **pointwise** operations applied to data arrays.

The simplest example of a stencil operator is given by

$$\psi := S(\phi) \text{ on } \mathbf{B}' \text{ , } S(\phi)_{\mathbf{i}} = \sum_{\mathbf{s} \in \mathcal{S}} a_{\mathbf{s}} \phi_{\mathbf{i} + \mathbf{s}},$$

where the coefficients $a_s \in \mathbb{T}$, S is a finite subset of \mathbb{Z}^D , and $B' \subseteq \cap_{s \in S}(B(\phi) - s)$. Such operators appear as finite difference approximations to constant-coefficient differential operators. For multilevel algorithms such as AMR and multigird, we will want more general versions of stencil operators corresponding to strided access through the data array. A more general form of such a stencil is given by

$$\psi := S(\phi) \text{ on } \mathbf{B}'$$

$$S(\phi)_{\mathbf{r}^d \mathbf{i} + \mathbf{t}} = \sum_{\mathbf{s} \in S} a_{\mathbf{s}} \phi_{\mathbf{r}^s \mathbf{i} + \mathbf{s}} , \mathbf{i} \in \mathbf{B}'$$
(3)

where $\mathbf{r}\mathbf{i} = (r_0i_0, \dots, r_{D-1}i_{D-1}) \in \mathbb{Z}^D$. Note that, if $\mathbf{r}^d \neq \mathbf{u}$, the application of the stencil assigns values to a strided subset of the data array on the left-hand side.

While the action of stencil on an a data array depend on the inputs, stencils themselves, as specified by the collection of offsets and weights $\{(s, a_s) : s \in \mathcal{S}\}$ and the input and output stride and output offset (r^s, r^d, t) have a mathematical meaning independent of the inputs. In particular, if $r^s, r^d = 1$, and t = 0, stencils can be added, multiplied by scalars, and composed to obtain new stencils.

$$S = tS_1 + S_2 \Leftrightarrow S(\phi)_i = \sum_{s \in S_1 \cup S_2} (ta_s^1 + a_s^2)\phi_{i+s}$$
(4)

$$S = S_1 \cdot S_2 \Leftrightarrow S(\phi)_i = \sum_{s \in \mathcal{S}} (\sum_{s_1, s_2 : s_1 + s_2 = s} a_{s_1}^1 a_{s_2}^2) \phi_{i+s} , \mathcal{S} = \{ s_1 + s_2 : s_1 \in \mathcal{S}_1, s_2 \in \mathcal{S}_2 \}.$$
 (5)

Algebraic operations and composition enables the construction of complex stencils from simpler ones as a symbolic preprocessing step.

Pointwise operators are defined using functions of one or more variables of the form (??). Given

$$F: \mathcal{T}_1 \times \cdots \times \mathcal{T}_P \to \mathcal{T}$$

we define F@, the pointwise operator derived from F, to be

$$\psi = F@(\phi^1, \dots, \phi^P) \text{ on } \mathbf{B}' \Leftrightarrow \psi_i = F(\phi_i^1, \dots, \phi_i^P) , i \in \mathbf{B}'$$

$$\mathbf{B}' \subseteq \mathbf{B}(\psi) \cap \mathbf{B}(\phi^1) \cap \dots \cap \mathbf{B}(\phi^P)$$
(6)

4 Proto Classes

There are four C++ classes that implement a representation of spatial discretizations on rectangular grids described above.

- Point represents points in \mathbb{Z}^D .
- Box represents rectangular subsets of \mathbb{Z}^D .

• BoxData<T,C,D,E> represents data arrays of the form

$$\phi: \mathbf{B} \Rightarrow \mathcal{T}, \mathcal{T}(\mathbb{T}, C, D, E).$$

BoxData is a templated class, with class templates specifying the values taken on by the array, and the dimensions of the range space \mathcal{T} given by C,D,E.

• Stencil is a class that defines stencils as self-contained objects.

We provide a more detailed summary of these classes below. The full documentation is contained in the Doxygen-annotated header files for Proto.

4.1 Point

A Point is a vector in \mathbb{Z}^D . Protouses Points to define locations in a grid as well as offsets between grid cells. The number of component axes of a Point - and all the objects which depend on Point - is determined from the compile-time constant DIM.

- Construction. Points can be constructed from C arrays of length DIM, and from integer tuple literals Point({1,2,1,2,1,2}). In the latter case, the number of elements in the integer tuple can be greater than DIM, with the ones exceeding the length being ignored. There are also static member functions that return a Point whose components are all zeros (Point::Zeros()), all ones (Point::Ones()), and the unit vector in the dth direction (Point::Basis(d), d = 0,..., DIM 1.
- Arithmetic Operators. Points have addition, componentwise multiplication, multiplication and division by an integer (in the latter case, with rounding toward $-\infty$).
- Logical Operators. p1 == p2, p1 != p2. The inequality operators e.g. p1 > p2 return true if they are true for each pair of components, i.e. the usual partial ordering on \mathbb{Z}^D .
- Indexing Operators. p[d], d = 0, ..., D 1. returns the d^{th} component of p. p[d] can appear as the left-hand side in an assignment.

4.2 Box

A Box is an D dimensional rectangle in \mathbb{Z}^D , defined by a pair of Points defining the low and high corners of the Box.

- <u>Constructors</u>. Box(low,high), where low, high are Points. If (high >= low) == false, then the Box is an empty Box.
- Accessors and Queries B1 == B2, B1 != B2, contains(Point a_pt), onBoundary(Point a_pt), empty() all return bools.

- Operators and Transformations. B1 & B2 returns the intersection of the two Boxes. coarsen, refine, shift and other transformation operations compute Boxes needed to construct BoxData targets for various structured-grid algorithms.
- <u>Iterators</u>. BoxIterator iterates over the Points in a Box. It is accessible using the standard iterator syntax: bx.begin() returns a BoxIterator for the Box bx initialized at the starting location; it.done() returns a bool telling whether the iterator has reached to end; and ++it increments the iterator.

4.3 BoxData

A BoxData<T,C,D,E> represents a data array defined on a Box domain of the form (??)

$$U: \mathbf{B} \to \mathcal{T}, \ \mathcal{T} = \mathcal{T}(C, D, E),$$

where C, D, and E are positive integers which define the sizes of *component axes* 0, 1, and 2 respectively. These values define the nature of data in a BoxData as shown below:

- \bullet : $C = D = E = 1 \rightarrow Scalar$
- : $C > 1, D = E = 1 \rightarrow \text{Vector}$ (1st Order Tensor) of length C
- : $C, D > 1, E = 1 \rightarrow C \times D$ Matrix (2nd Order Tensor)
- : $C, D, E > 1 \rightarrow C \times D \times E$ 3rd Order Tensor

BoxData has an accompanying class Interval<C,D,E> which represents the analog of Box in *component space*. Interval facilitates copy and slicing operations on BoxDatas. Operations on BoxData include the following:

• Construction.

BoxData(const Box& a_bx), define(const Box& a_bx) define a BoxData over the Box a_bx. We can also control whether the data is allocated from the heap (defineMalloc) or from a specialized stack manager (defineStack) that provides a low-overhead way of allocating temporaries; the default is the latter.

Copy construction and assignment are deleted. However, move construction and assignment is supported: BoxData (BoxData< T, C, D, E > &&a_src), BoxData& operator= (BoxData< T, C, D, E > &&a_src). iota creates a BoxData<T,DIM> from a Box and a step size of type T that represents a space of position vectors in \mathbb{T}^D .

• Algebraic Operations. operator {+,*,-,/} (const BoxData& a_bd) returns a BoxData on the intersection of the Boxes on which the two inputs are defined. operator {+=,*=,-=,/=} (const BoxData& a_bd) computes the same set of values,

but updates the left-hand side in place. We also define operator() {+=,*=,-=,/=}() (T a_t) to apply the operator to each value in the BoxData, and update the left-hand side in place. setVal(T a_t) sets all of the values of the BoxData to a_t. min, max, and absMax: Computes the min, max, or absolute max of a BoxData.

• Slicing and Shifting. Operations on BoxDatas are specific to the type; in particular, they cannot be performed on a BoxData with one set of component ranges to produce a BoxData with a different set of component ranges. For example,

creates a scalar-valued BoxData that points to the slice corresponding to component (a_c,a_d,a_e). The resulting BoxData can then be used in functions taking scalar-valued BoxDatas. Similarly, the function

creates a BoxData with the same data pointer, but the Box offset by a_shift.

Var, Param, and Forall

One of the two types of aggregate operations on BoxDatas is pointwise application of functions (??). This is represented in Protousing forall. For example, we want to compute A' = F@A, where

$$A: \boldsymbol{B_A} \to \mathcal{T} , F: \mathcal{T} \to \mathcal{T}'$$

This is done in Proto by defining the function F that represents the function F.

```
void
F(Var<T,Cprime>& AprimePoint, const Var<T,C>& APoint>
{
AprimePoint(0) = APoint(1);
AprimePoint(1) = APoint(2) * APoint(3);
...
}
```

This is then applied at all points $p \in B_A$ using forall

```
BoxData<T,C,D,E> A = ...;
auto Aprime = forall<T,Cprime>(F,A);
```

Thus the class Var<T,C,D,E> is the value type of a BoxData, when the latter is viewed as a map from a Box to $\mathbb{T}^C \times \mathbb{T}^D \times \mathbb{T}^E$, and the pointwise function F is written in terms of Vars as input and output. More generally the signature of a forall function is given as follows.

```
forall<T,C,D,E>forall(const Func & a_F, Srcs &... a_srcs)
```

where the first argument is the function F that is to be applied pointwise, and the following arguments are set of BoxDatas and scalar parameters. The matching signature for F is

where the first argument is the output value, and Typej is a type corresponding to the j^{th} entry in the forall src ... list: if the j^{th} entry is a scalar type, then Typej = Tj; if the j^{th} entry is of type BoxData<Tj,Cj,Dj,Ej>, then Typej = Var<Tj,Cj,Dj,Ej>. In this case, the return BoxData<T,C,D,E> from forall is defined on the intersection of all the BoxData.box() in the argument list. There are also variations of forall that enable restriction of the result to an input Box, and allows an argument to F corresponding to the Points in a Box. Thus forall is a very powerful abstraction; for example, when combined with alias on BoxData it can be used to implement stencil operations, including nonlinear stencils, e.g. that occur in limiters for hyperbolic PDE. However, for the case of constant-coefficient stencils, we provide a specialized class Stencil, described below.

4.4 Stencil

A Stencil<T> is a object used to define and implement the operations described in ??, with coefficients of type T. Typically, Stencils are constructed using a companion class Shift which represents the grid shifts associated with a stencil operation. In addition, Stencil implements the operations (??), (??). Stencils are then applied to BoxData objects to update existing ones, or produce new ones.

• <u>Construction and Definition</u>. Default-constructed **Stencils** are empty, containing no offsets or definitions. Stencil has non-default constructors, but they are mostly not used by applications. The most common way to construct a **Stencil** is as a (sum of) **Shifts** multiplied by weights.

```
Point pt = ...; T wgt = ...; Stencil<T> = wgt*Shift(pt);
```

In addition, Stencils can be constructed using the operators +, * that implement the corresponding operations in (??), (??).

```
Stencil<T> S1= ...; Stencil<T> S2 = ...; T wgt = ...;
auto SVec = S1 + wgt*S2; auto SComp = S1*S2;
```

There are a number of Stencils precomputed and accessible through member functions of the class Stencil, including Stencil<T>::Derivative(...),

Stencil<T>::Laplacian(...), and various interpolation Stencils useful finite volume applications. We provide support for strided Stencils, as in (??), either in the constructor, or by setting r^s , r^d , or d using the member functions srcRatio(), destRatio(), destShift(), respectively.

• Applying Stencils. Stencils can be applied to a BoxData to update the values in an existing BoxData.

```
BoxData<T> A1 = ...;BoxData<T> A2 = ...;Stencil<T> L = ...;T wgt = ...;
A1 |= L(A2);
A1 += L(A2,wgt);
```

In the first case, the values in A1 are overwritten by those given by L(A2). In the second case, the values in A1 are incremented by those given by L(A2)*wgt. In both cases, the operations are performed on the points $pt \in A2.box()\&L(A2).box()$. Stencil application also can be used with assignment to create a new BoxData.

```
BoxData<T> A1 = ...; Stencil<T> L = ...; T wgt = ...; auto A2 = L(A2, wgt);
```

4.5 Interface to Chombo

Proto is designed for a shared memory environment. To use Proto in a distributed memory environment, we use the Chombo4 infrastructure. Chombo4 uses Chombos LevelData to distribute data. Proto has data holders for both device-based and host-based data. Currently, communication and I/O are done on the host. Chombo4 provides LevelBoxData, a class which wraps LevelData<BoxData<...> and provides functions to move data between the host and the device.

5 Examples

5.1 Point Relaxation

The code example ?? below implements one iteration of point Jacobi for L^h , the standard 5/7 point, second-order accurate discretization of the Laplacian on a grid of mesh spacing h

$$\phi: D \to \mathbb{R} , \rho: D_0 \to \mathbb{R}$$

 $\phi:=\phi + \lambda(L^h(\phi) - \rho) , \lambda = \frac{h^2}{4D}.$

Listing 1: Point Jacobi Relaxation for Poisson

The second example is that of a fourth-order accurate evaluation of the right-hand side for a finite-volume discretization of the compressible Euler equations, suitable for use in a method of lines integrator.

$$\langle U \rangle : \boldsymbol{B} \to \mathbb{R}^{\boldsymbol{D}+2} , \langle R \rangle : \boldsymbol{B}_0 \to \mathbb{R}^{\boldsymbol{D}+2} , \boldsymbol{B} \supseteq grow(\boldsymbol{B}_0, 5)$$

$$\bar{W} = \mathcal{C}(., \gamma) @ \langle U \rangle)$$

$$U = \bar{U} - \frac{h^2}{24} \Delta^h(\langle U \rangle)$$

$$W = \mathcal{C}(., \gamma) @ (U)$$

$$\langle W \rangle = W + \frac{h^2}{24} \Delta^h(\bar{W})$$

$$\langle R \rangle = 0$$

for d = 0, ... D - 1:

$$\begin{split} W_L &= D_L^d(\langle W \rangle) \;, \, W_R = D_R^d(\langle W \rangle) \\ \langle W \rangle_{face} &= \mathcal{U}(.,.,\gamma)@(W_L,W_R) \\ \bar{F}_{face} &= \mathcal{F}(.,d,\gamma)@(\langle W \rangle_{face}) \\ W_{face} &= \langle W \rangle_{face} + \frac{h^2}{24} \Delta^{h,d,\perp}(\langle W \rangle_{face}) \\ F_{face} &= \mathcal{F}(.,d,\gamma)@(W_{face}) \\ \langle F \rangle_{face} &= F_{face} + \frac{h^2}{24} \Delta^{h,d,\perp}(\bar{F}_{face}) \\ \langle R \rangle + = \frac{1}{h} (I - (\mathcal{S}^d)^{-1})(\langle F \rangle_{face}). \end{split}$$

Here, the functions C, U, and \mathcal{F} are, respectively, the mapping from conservative to primitive variables, an approximate solution to the Riemann problem given left and right state, and the flux in the d direction given a value for the primitive variables. The stencil operators Δ^h , $\Delta^{h,d,\perp}$, and $D^d_{\{L,R\}}$ are, respectively: the classical 5/7 point second-order discrete Laplacian; the second-order Laplacian minus the second differences in the d^{th} direction; and the interpolation of averages over d faces given cell averages using an upwind-biased fifth-order operator.

Listing 2: High-order upwind right-hand side for compressible Euler

```
void EulerOp::operator()(BoxData<Real,NUMCOMPS& a_R,</pre>
                               const BoxData<Real ,NUMCOMPS& a_Uave)
3
     a_Rhs.setVal(0.0);
5
     Real gamma = s_gamma;
6
     auto W_bar = forall < Real , NUMCOMPS>(consToPrim , a_Uave , gamma);
8
     auto U = s_deconvolve(a_U);
9
     auto W = forall < Real, NUMCOMPS>(consToPrim, U, gamma);
10
     auto W_ave = s_laplacian(W_bar, 1.0/24.0);
11
     W_{ave} += W;
12
13
     for (int d = 0; d < DIM; d++)
14
       auto W_ave_low = s_interp_L[d](W_ave);
       auto W_ave_high = s_interp_H[d](W_ave);
17
       auto W_ave_f = forall < Real, NUMCOMPS>
18
                        (upwindState, W_ave_low, W_ave_high, d, gamma);
19
20
```

```
auto F_bar_f = forall <Real ,NUMCOMPS>(getFlux , W_ave_f , d , gamma); auto W_f = s_deconvolve_f [d] ( W_ave_f ); auto W_f = W_ave_f; auto F_ave_f = forall <Real ,NUMCOMPS>(getFlux , W_f , d , gamma); auto F_ave_f += s_laplacian_f [d] ( F_bar_f , 1.0 / 24.0 ); a_Rhs += s_divergence [d] ( F_ave_f ); } a_Rhs *= -1./s_dx; }
```

Listing 3: Pointwise functions for Euler

```
:: Proto:: Var<Real, NUMCOMPS State;
  typedef
  PROTO_KERNEL_START
  void
  consToPrimF (State&
                                 a_W,
                const State&
                                 a_U,
5
                Real
                               a_gamma)
6
     Real rho = a_U(0);
8
     Real v2 = 0.0;
9
     Real gamma = a\_gamma;
    a_W(0) = rho;
11
     for (int i = 1; i \leq DIM; i++)
13
       Real v;
14
       v = a_U(i) / rho;
       a_{-}W(i) = v;
       v2 + v*v;
18
     a_W(NUMCOMPS-1) =
19
               (a_U(NUMCOMPS-1) - .5 * rho * v2) * (gamma - 1.0);
20
21
  PROTO_KERNEL_END(consToPrimF, consToPrim)
22
  PROTO_KERNEL_START
   void upwindStateF(State& a_out,
24
                       const State& a_low,
25
                       const State& a_high,
26
                       int
                              a_dir,
27
                       Real a_gamma)
28
   \{\ldots\}
29
  PROTO_KERNEL_END(upwindStateF, upwindState)
```

```
PROTO_KERNEL_START

void getFluxF(State& a_F,

const State& a_W,

int a_dir,

Real a_gamma)

{...}

PROTO_KERNEL_END(getFluxF, getFlux)
```