Public Resources for Bioinformatics

- Databases
- Analysis Tools

Observe: List of databases and service at NCBI, EBI, KEGG, and Ensembl.

Public Resources (II) – Analysis tools

- Web-based analysis tools – easy to use, but often with less customization options.
- Stand-alone analysis tools – requires installation and configuration, but provides more customization options.
- Commercial analysis tools
- Scripting for bioinformatics projects

web-based tools

Practice –design QPCR primers for IL-6 or your gene.

Stand-alone tools 1.

Rules of the thumb:

- **Make a folder for each program.**
- **Make a sub-folder for input/output if necessary.**
- **Read the instructions before installation.**

Stand-alone tools 3.

Command line applications:

- **Accounts for a large number of high-quality, sophisticated programs.**

Practice – (install and) run standalone blast in your own computer

Pet Projects:

Searching for potential ortholog of IL6 in the *Drosophila* genome

Practice – Install the blast program (1)

1. Read the manuals, download the appropriate BLAST executable file.
2. Run the installation. Inspect the folder following installation.
3. Inspect the contents of the doc and bin subfolders following the installation.
4. Verify the installation by executing the “makeblastdb” in a terminal.

Practice – Install the blast program (2)

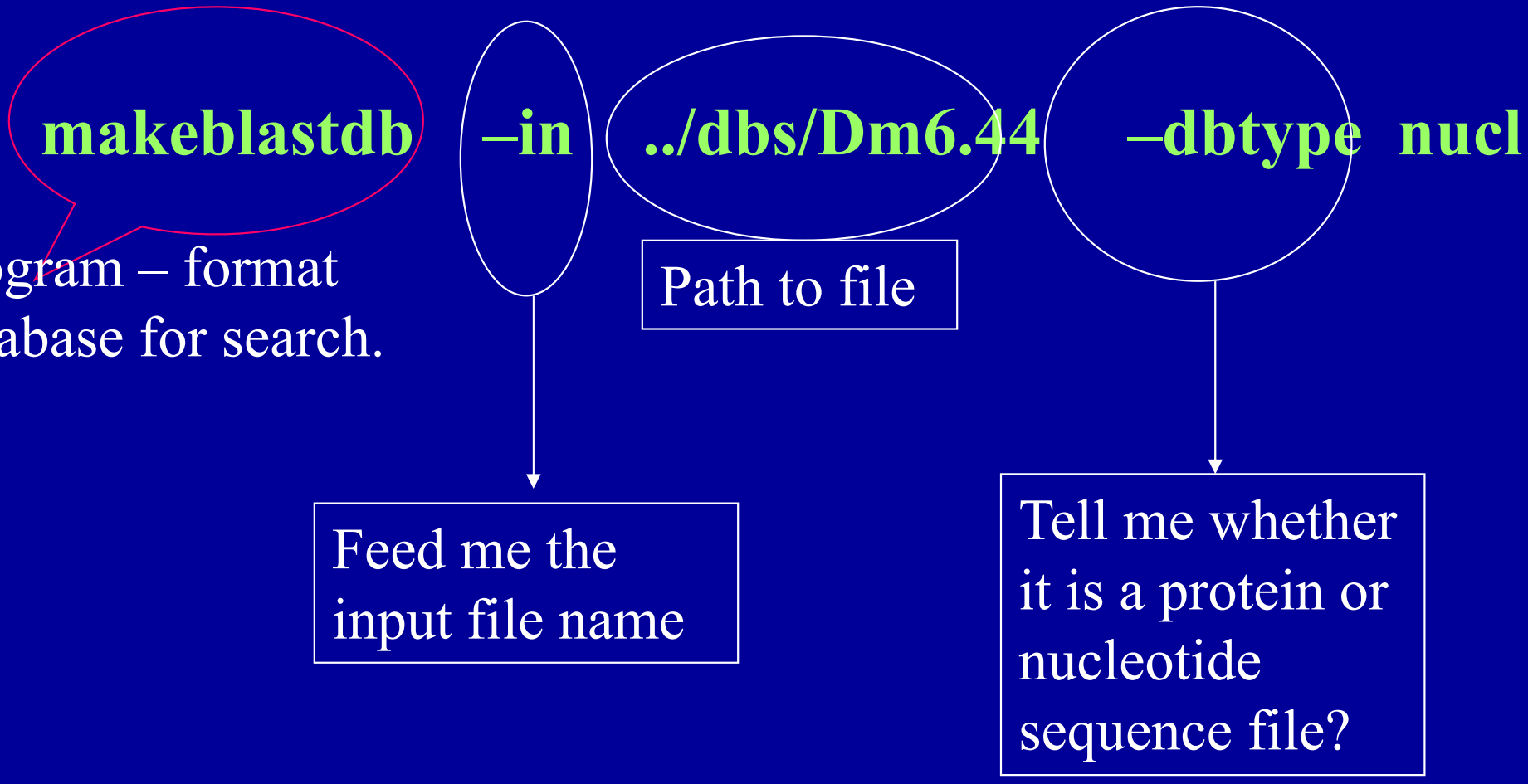
5. Make a /blast folder in your home/GMS6014 folder.
6. Add three more folders to your /blast directory, “/query”, “/dbs”, and “/out”.
7. Start a terminal at the blast folder.

Practice -- BLAST search in your own computer

1. **Download data file from the course web page, or Ensemble. Save in the blast\dbs folder.**
2. **Start a CMD window (or Terminal in Mac), navigate to the C:\GMS6014\blast folder.**
3. **At the prompt "C:\GMS6014\blast\bin>" type the command "makeblastdb –in ../dbs/Dm6.44 –dbtype nucl"* -- format the dataset for the program.**
4. **Compose the query sequence save as "3LL6.txt" in the "blast\query\" folder.**
5. **Initiated the search by typing "tblastn –db ../dbs/ Dm6.44 –query ../query/3IL6.txt –out ../out/myblast.html –html"**

*Command syntax may be different depending on platform and setup

What's in a command?



For more info, refer to the "user manual" file in the blast\doc folder.

Advantages of Running BLAST at Your Own Machine

- Do it at any time, no waiting on the line.
- Search for multiple sequences at once.
- Search a defined data set.
- Automate Blast analysis.
- Combine Blast with other analysis.
- …..

BLAST is a program implemented in C/C++

```
void BlastTickProc(Int4 sequence_number, BlastThrInfoPtr thr_info)
{
    if(thr_info->tick_callback &&
       (sequence_number > (thr_info->last_db_seq + thr_info->db_incr))) {
        NlmMutexLockEx(&thr_info->callback_mutex);
        thr_info->last_db_seq += thr_info->db_incr;
        thr_info->tick_callback(sequence_number, thr_info->number_of_pos_hits);
    }
    return;
}
/*
     Sends out a message every PERIOD (i.e., 60 secs.) for the index.
     THis function runs as a separate thread and only runs on a threaded
     platform.
```

Should I care ?

If you care:

1.) Data structure and Algorithm

SEQ
- char: name
- char: sequence
- int: seq_length

Identify the best alignment for two sequences (p69-73)

```
Seq1: MA-DSV—WC..
Seq2: MALD-IHWS..
```

Programming language comparison

Translation : C

```
/* TRANSLATION: 3 or 6 frame translate cDNA sequences
          */
//---------------------------------------------------------------------------
#include "translation.hpp"

int main(int argc, char **argv)
{   int num_seq=0;
          char string[MAXLINE];
   DSEQ * dseq;


          infile.getline (string,MAXLINE);
   if (string[0]=='>') strncpy (dbname,string,MAXLINE);
   while (!infile.eof())
   {   dseq=Get_Lib_Seq ();
      if (dseq->reverse==0)
         Translation (&dseq->name[1], dseq->seq);
      else
         Translation (&dseq->name[1], dseq->r_seq);
          num_seq++;
      if (num_seq%1000==0)
      {   cout<<num_seq<<endl;
         cout<<dseq->name<<endl;
      }
      delete dseq;
   }

   infile.close();
   outfile.close();
   cout<<num_seq<<" translated"<<endl;
   getch();
          return 0;
}

DSEQ* Get_Lib_Seq()
{   int i,n;
   char str[MAXLINE];
   DSEQ* dseq;
   n = 0;
   dseq=new DSEQ;
   strcpy (dseq->name, dbname);
```

Translation : Python

```
f#Translation -- read from fasta DNA file and translate into
three frames

#

import string

from Bio import Fasta

from Bio.Tools import Translate

from Bio.Alphabet import IUPAC

from Bio.Seq import Seq

ifile = "S:\\Seq\\test.fasta"

parser = Fasta.RecordParser()

file =open (ifile)

iterator = Fasta.Iterator (file, parser)

cur_rec = iterator.next()

cur_seq = Seq (cur_rec.sequence,IUPACUnambiguousDNA())

translator = Translate.unambiguous_dna_by_id[1]

translator.translate (cur_seq)
```

Programming languages and platforms

Efficiency, Power	Simplicity, Fast Dev.
C/C++	Perl - Bioperl
Java - Biojava	Python - Biopython